10080926

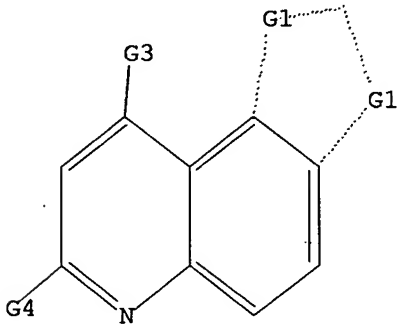
=> d his

(FILE 'HOME' ENTERED AT 17:58:00 ON 12 APR 2005)

FILE 'REGISTRY' ENTERED AT 17:58:05 ON 12 APR 2005
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 1 S L2
L4 70 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 18:00:43 ON 12 APR 2005
L5 4 S L4

=> d l2
L2 HAS NO ANSWERS
L2 STR



G1 C,N

G2

G3 C,O,S,N,X,CN

G4 O,S,N,Cl,Br,F,I,CN

Structure attributes must be viewed using STN Express query preparation.

=> d 1-4 bib abs hitstr

L5 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:658121 CAPLUS
DN 137:201294
TI Preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compounds as androgen receptor modulators
IN Zhi, Lin; Van Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Higuchi, Robert I.
PA Ligand Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002066475	A2	20020829	WO 2002-IB537	20020223
	WO 2002066475	A3	20030123		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002183346	A1	20021205	US 2002-80926	20020222
CA 2434299	AA	20020829	CA 2002-2434299	20020223
EP 1363909	A2	20031126	EP 2002-702589	20020223

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

BR 2002007549	A	20040803	BR 2002-7549	20020223
JP 2004524309	T2	20040812	JP 2002-565989	20020223
PRAI US 2001-271189P	P	20010223		
WO 2002-IB537	W	20020223		

OS MARPAT 137:201294
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title nonsteroidal tricyclic compds. I-VIII [wherein R1 = H, halo, NO2, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl or heteroalkyl; R2 = H, halo, Me, CF3, CHF2, CH2F, CF2Cl, CN, CF2OR12, CH2OR12, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, or alkynyl; R3-R8 = independently H, halo, OR12, NR12R13, SO0-2R12, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, (hetero)aryl, or arylalkyl; or R3R5 or R5R7 = a bond; or C2R4R6 or C2R6R8 = (un)substituted carbocyclic or heterocyclic ring; R9 and R10 = independently H, halo, CN, OR12, NR12R13, Cm(R12)2mOR13, SO0-2R12, NR12COR13, or (un)substituted (halo)alkyl, heteroalkyl, or arylalkyl; R11 = H, halo, CN, OR14, NR14R15, SO0-2R14, CH2R14, COR14, CO2R14, CONR13R14, or (un)substituted (halo)alkyl or heteroalkyl; R12 and R13 = independently H or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, or (hetero)aryl; R14 = H, COR15, CO2R15, CONR15R16, or (un)substituted (halo)alkyl, heteroalkyl, or (hetero)aryl; R15 and R16 = independently H or (un)substituted (halo)alkyl, or heteroalkyl; W = O or S; X = O, S, or NR14; Y = O, S, NR12, NOR12, or CR12R13; Z = O, S, or NR12; n = 0-2; m = 0-2; or pharmaceutically acceptable salts thereof] were prepared as modulators of androgen receptors. For example, cyclization of 6-hydrazino-4-trifluoromethylquinolin-2(1H)-one with 3-pentanone afforded the cis-5,6-dihydro-7H-pyrrolo[3,2-f]quinolin-2(1H)-one. Oxidation with DDQ in CH2Cl2 gave 6-ethyl-5-methyl-7-(2,2,2-trifluoroethyl)-4-trifluoromethyl-1H-pyrrolo[3,2-f]quinolin-2(1H)-one (IX). The latter exhibited 76% androgen receptor agonist efficacy with a potency (EC50) of 7.6 nM relative to dihydrotestosterone in co-transfection assays using CV-1 cells and displayed androgen receptor binding activity (IC50) of 1.7 nM. Pharmaceutical compns. and formulations of IX are also disclosed. I-VIII are useful for the treatment of acne, male-pattern baldness, impotence, sexual dysfunction, wasting disease, hirsutism, hypogonadism, prostatic hyperplasia, osteoporosis, cancer cachexia, and hormone-dependent cancers (no data). Pharmaceutical compns. and formulations of IX are also disclosed.

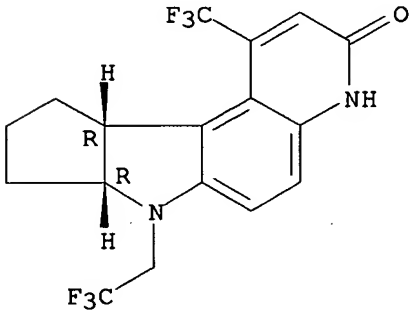
IT **453592-26-2P**
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical

process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-26-2 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



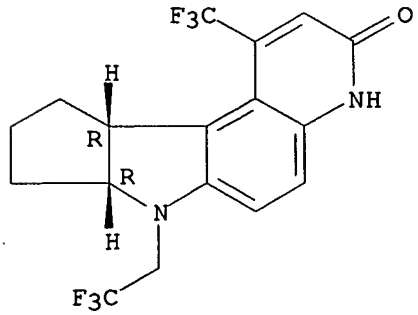
IT **453592-85-3P 453592-86-4P**

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-85-3 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(+)- (9CI) (CA INDEX NAME)

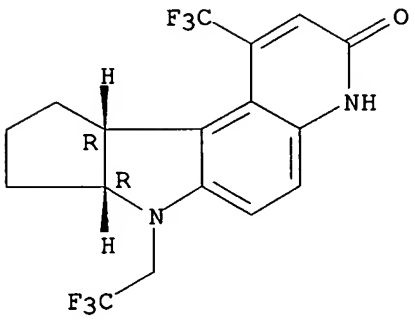
Rotation (+). Absolute stereochemistry unknown.



RN 453592-86-4 CAPLUS

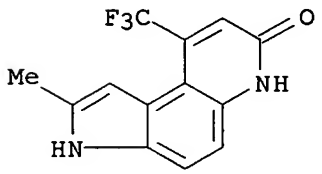
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

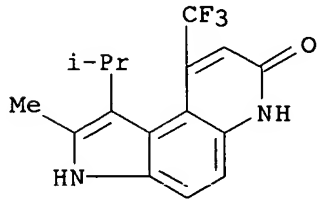


IT **453592-19-3P 453592-20-6P 453592-22-8P**
453592-24-0P 453592-25-1P 453592-30-8P
453592-39-7P 453592-41-1P 453592-46-6P
453592-47-7P 453592-52-4P 453592-53-5P
453592-54-6P 453592-57-9P 453592-60-4P
453592-71-7P 453592-72-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

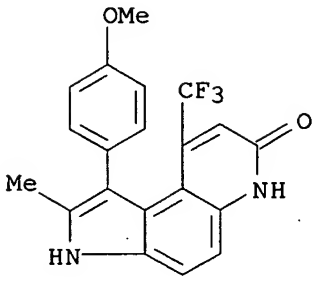
RN 453592-19-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



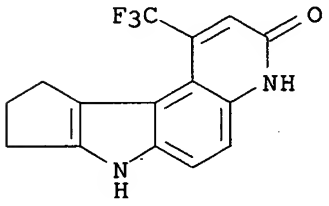
RN 453592-20-6 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(1-methylethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



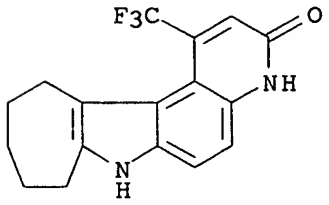
RN 453592-22-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-24-0 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)

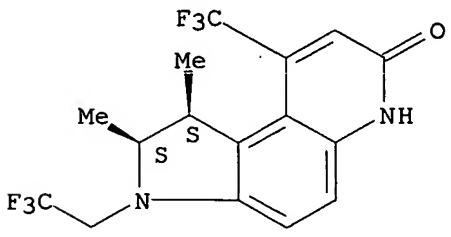


RN 453592-25-1 CAPLUS
CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10,11,12-hexahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



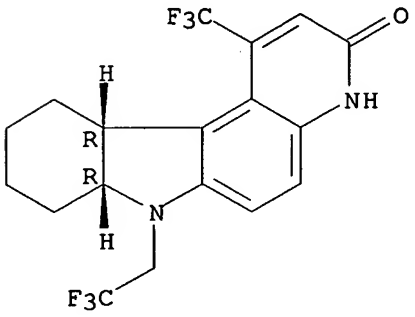
RN 453592-30-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



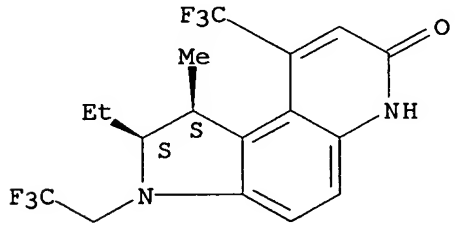
RN 453592-39-7 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7,7a,8,9,10,11,11a-octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,11aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



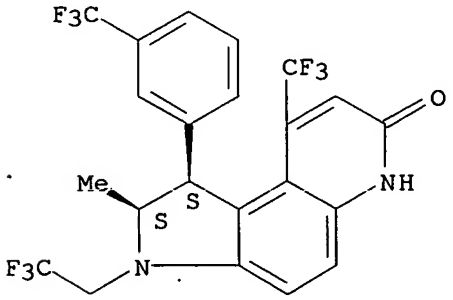
RN 453592-41-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-1,2,3,6-tetrahydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



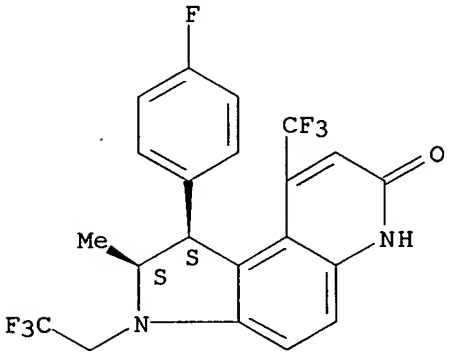
RN 453592-46-6 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

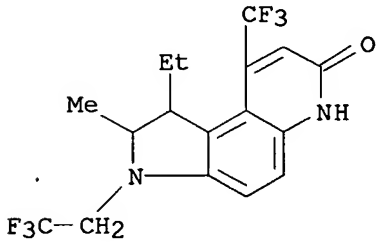


RN 453592-47-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

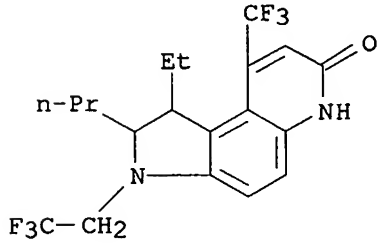
Relative stereochemistry.



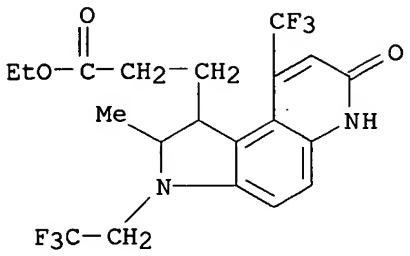
RN 453592-52-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



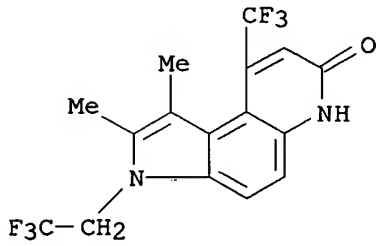
RN 453592-53-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



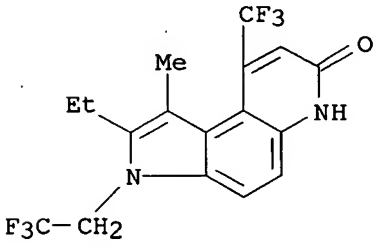
RN 453592-54-6 CAPLUS
CN 1H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 2,3,6,7-tetrahydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



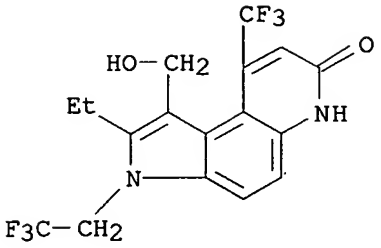
RN 453592-57-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



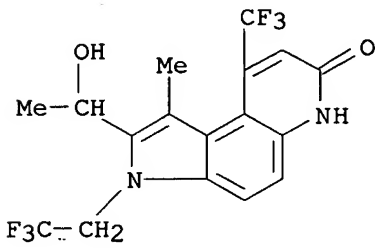
RN 453592-60-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-71-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-(hydroxymethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

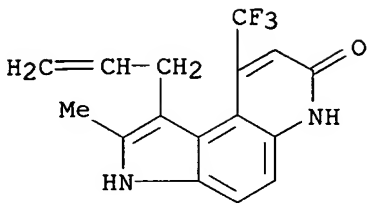


RN 453592-72-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-hydroxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

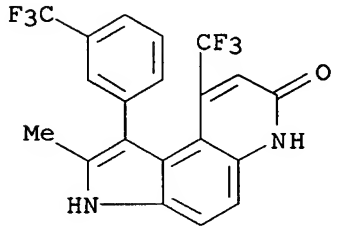


IT **453592-21-7P 453592-23-9P 453592-28-4P**
453592-32-0P 453592-33-1P 453592-34-2P
453592-35-3P 453592-36-4P 453592-37-5P
453592-38-6P 453592-40-0P 453592-42-2P
453592-43-3P 453592-44-4P 453592-45-5P
453592-48-8P 453592-49-9P 453592-50-2P
453592-51-3P 453592-59-1P 453592-61-5P
453592-62-6P 453592-63-7P 453592-64-8P
453592-65-9P 453592-67-1P 453592-68-2P
453592-69-3P 453592-73-9P 453592-74-0P
453592-75-1P 453592-76-2P 453592-77-3P
453592-78-4P 453592-79-5P 453592-80-8P
453592-82-0P 453592-83-1P 453592-84-2P
453593-25-4P 453593-26-5P 453593-30-1P
453593-31-2P 453593-32-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-21-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

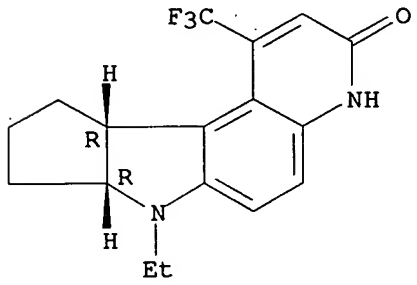


RN 453592-23-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



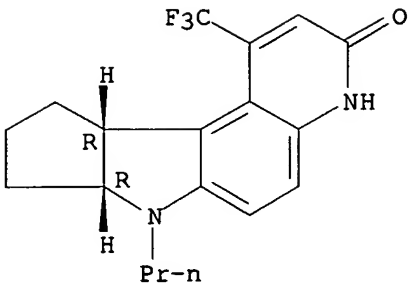
RN 453592-28-4 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-ethyl-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



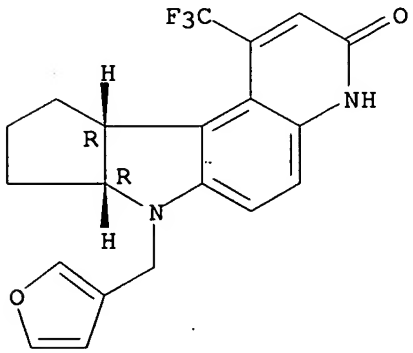
RN 453592-32-0 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-propyl-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



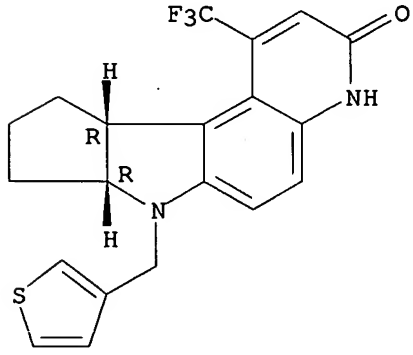
RN 453592-33-1 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(3-furanylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 453592-34-2 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(3-thienylmethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

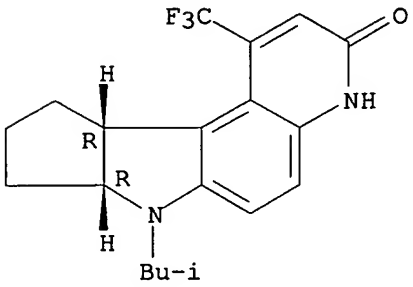
Relative stereochemistry.



RN 453592-35-3 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2-methylpropyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX

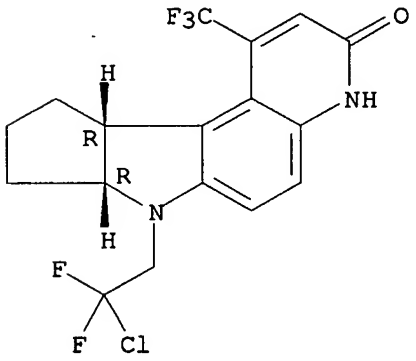
NAME)

Relative stereochemistry.



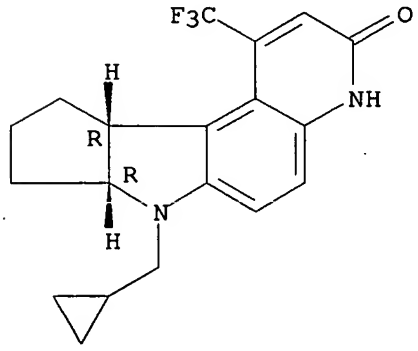
RN 453592-36-4 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2-chloro-2,2-difluoroethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



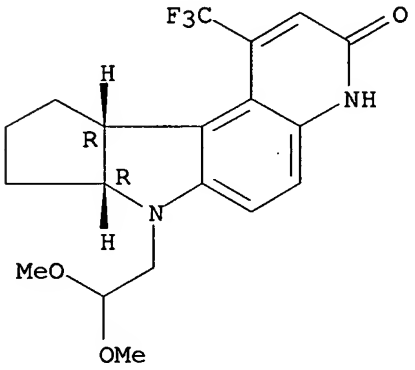
RN 453592-37-5 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(cyclopropylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



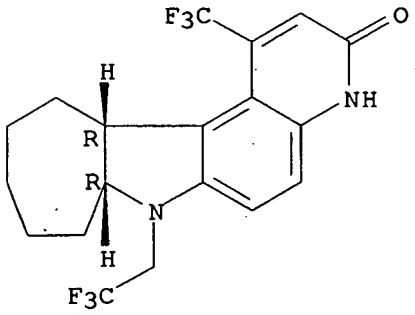
RN 453592-38-6 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2,2-dimethoxyethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



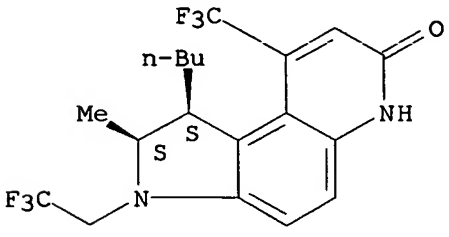
RN 453592-40-0 CAPLUS
CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,11,12,12a-octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,12aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



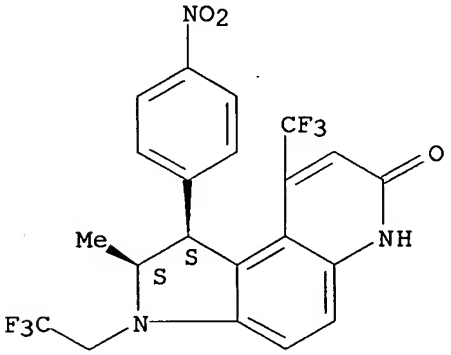
RN 453592-42-2 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-butyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



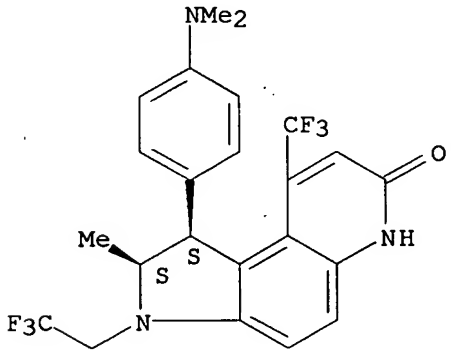
RN 453592-43-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(4-nitrophenyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



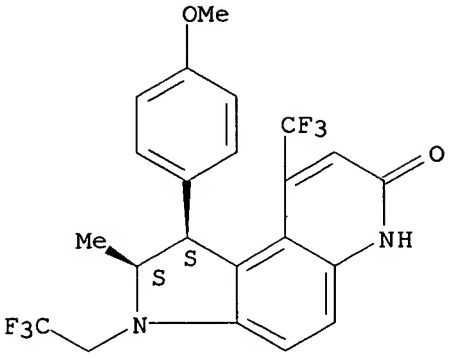
RN 453592-44-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[4-(dimethylamino)phenyl]-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

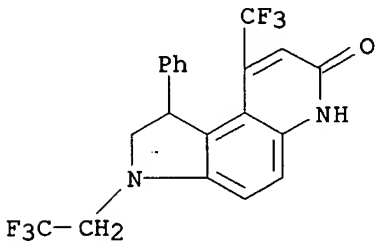


RN 453592-45-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

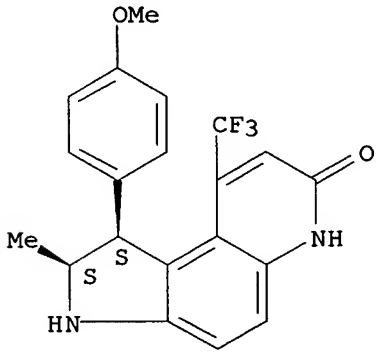


RN 453592-48-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-phenyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



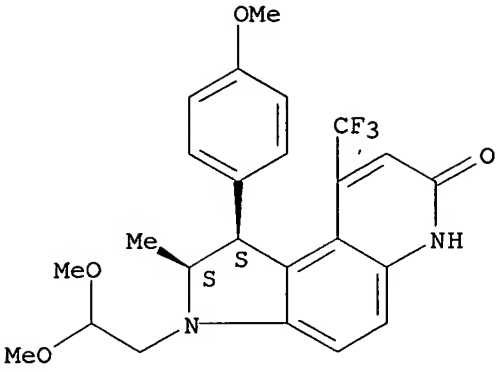
RN 453592-49-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



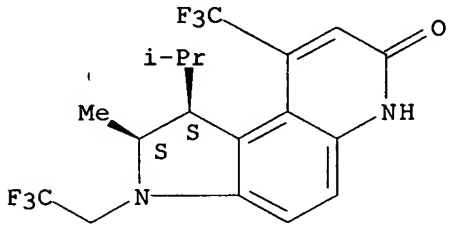
RN 453592-50-2 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-dimethoxyethyl)-1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

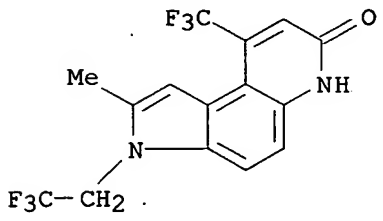


RN 453592-51-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(1-methylethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

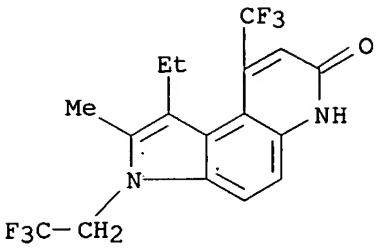
Relative stereochemistry.



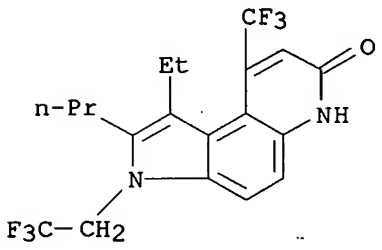
RN 453592-59-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



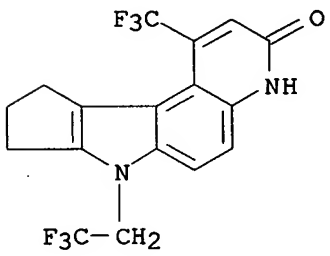
RN 453592-61-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



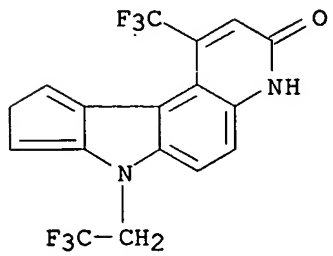
RN 453592-62-6 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



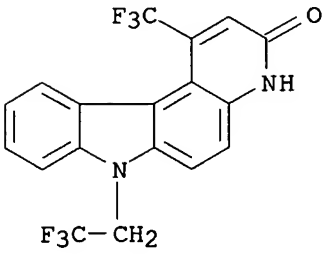
RN 453592-63-7 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



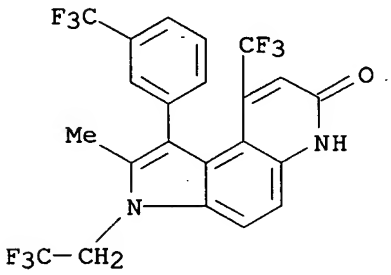
RN 453592-64-8 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,9-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



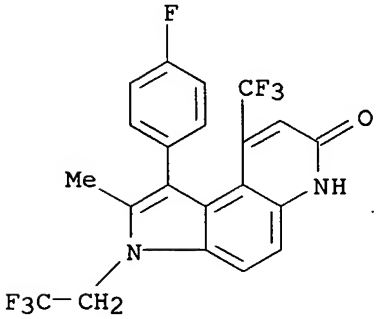
RN 453592-65-9 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



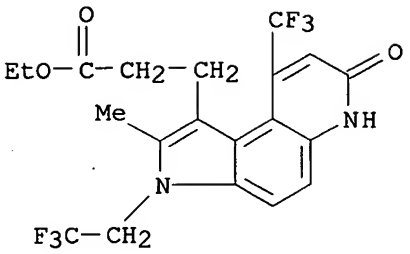
RN 453592-67-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



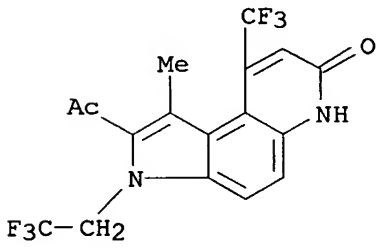
RN 453592-68-2 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



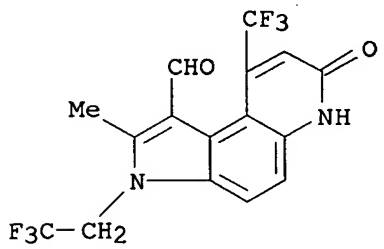
RN 453592-69-3 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



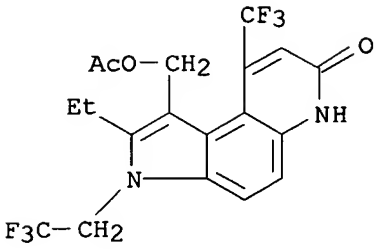
RN 453592-73-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-acetyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



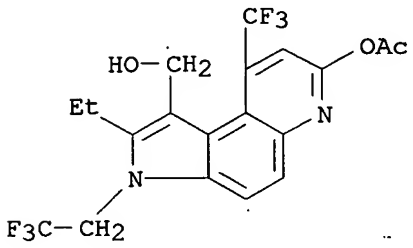
RN 453592-74-0 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-1-carboxaldehyde, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



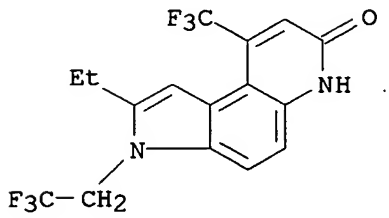
RN 453592-75-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[(acetyloxy)methyl]-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



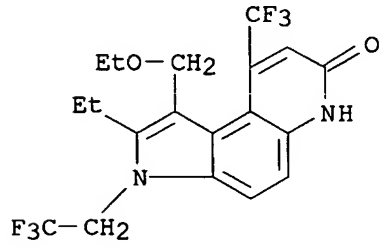
RN 453592-76-2 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-1-methanol, 7-(acetyloxy)-2-ethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



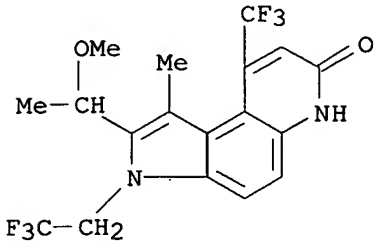
RN 453592-77-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



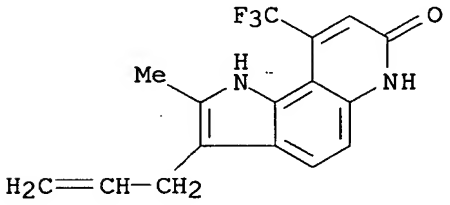
RN 453592-78-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(ethoxymethyl)-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



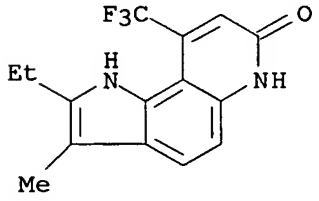
RN 453592-79-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-methoxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



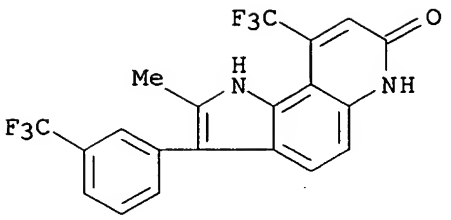
RN 453592-80-8 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-3-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



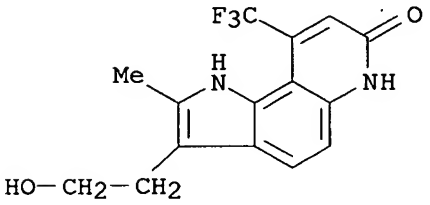
RN 453592-82-0 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 2-ethyl-1,6-dihydro-3-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



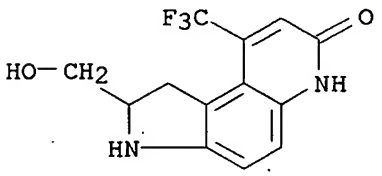
RN 453592-83-1 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-9-(trifluoromethyl)-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



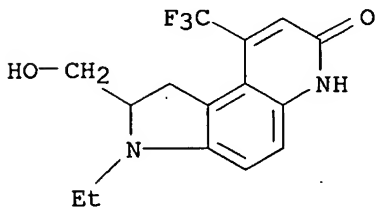
RN 453592-84-2 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-3-(2-hydroxyethyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



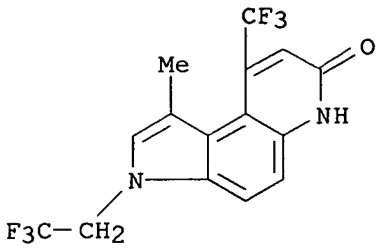
RN 453593-25-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



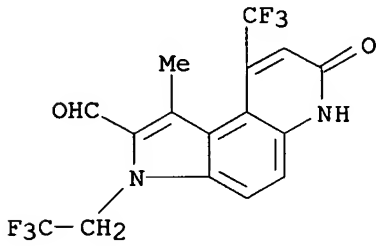
RN 453593-26-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-ethyl-1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



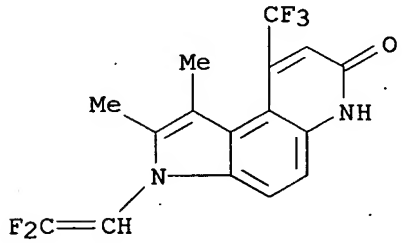
RN 453593-30-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-31-2 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-2-carboxaldehyde, 6,7-dihydro-1-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



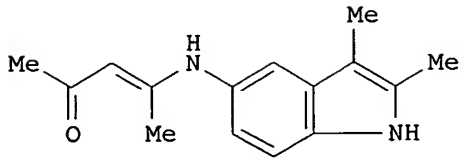
RN 453593-32-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-difluoroethenyl)-3,6-dihydro-1,2-dimethyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:455695 CAPLUS
DN 131:213835
TI Reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines
AU Yamashkin, S. A.; Trushkov, I. V.; Tomilin, O. B.; Terekhin, I. I.; Yurovskaya, M. A.
CS Mordovian State Pedagogical Institute, Sarinsk, 430007, Russia
SO Chemistry of Heterocyclic Compounds (New York)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9), 1050-1065
CODEN: CHCCAL; ISSN: 0009-3122
PB Consultants Bureau

10080926

DT Journal
LA English
GI

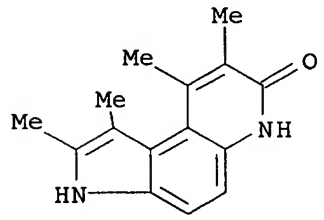


I

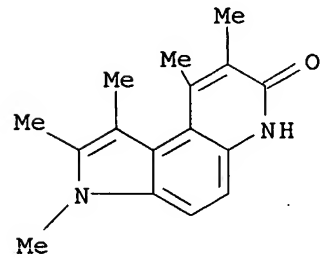
AB The concept of regioorientation is proposed for the annelation of the pyridine ring with the participation of 5-, 6-, and 7-aminoindoles (e.g. ,I). The conclusions based on the exptl. data are supported by semiempirical AM1, PM3, and MNDO quantum-chemical calcns.

IT **243669-00-3 243669-02-5 243669-06-9**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines)

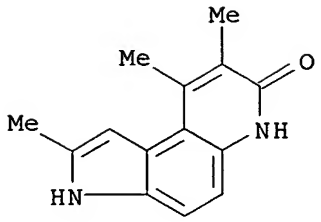
RN 243669-00-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,8,9-tetramethyl- (9CI) (CA INDEX NAME)



RN 243669-02-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,3,8,9-pentamethyl- (9CI) (CA INDEX NAME)

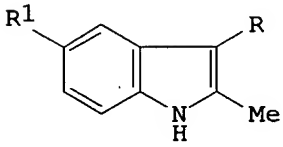


RN 243669-06-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2,8,9-trimethyl- (9CI) (CA INDEX NAME)

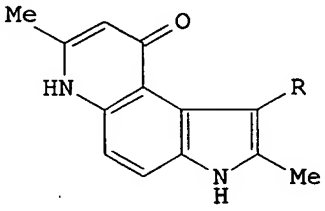


RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

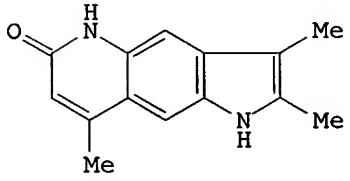
L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:438395 CAPLUS
DN 99:38395
TI Synthesis of pyrroloquinolones
AU Yamashkin, S. A.; Yudin, L. G.; Kost, A. N.
CS Mosk. Gos. Univ., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1983), (4), 493-7
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 99:38395
GI



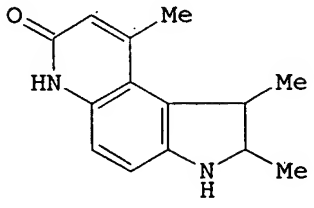
I



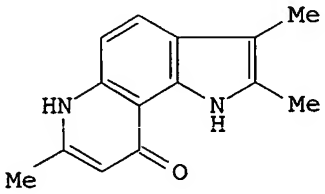
II



III



IV



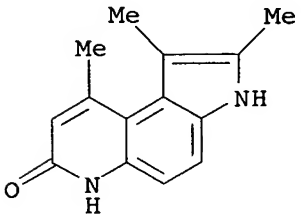
V

AB Intramol. cyclocondensation of I (R = Me, H; R1 = EtO2CCH:CMeNH) by refluxing in biphenyl gave 89 and 95% pyrroloquinolines II. Similarly, refluxing I (R = Me, R1 = MeCOCH2CONH) in F3CCO2H gave a mixture containing III and IV. Refluxing I (R = Me, R1 = EtO2CCH:CMeNH in the 6 position) with biphenyl gave 90% V.

IT **86269-88-7P 86269-91-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

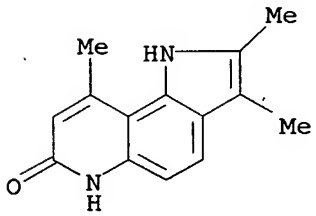
RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)



RN 86269-91-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2,3,9-trimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1948:32006 CAPLUS

DN 42:32006

OREF 42:6783h-i,6784a-i,6785a-i,6786a-i,6787a-i,6788a-e

TI Orienting experiments on the reaction mechanism of aromatic bicyclic compounds

AU Huisgen, Rolf

CS Univ. Munich, Weilheim, Germany

SO Ann. (1948), 559, 101-52

DT Journal

LA Unavailable

OS CASREACT 42:32006

GI For diagram(s), see printed CA Issue.

AB A comprehensive monograph dealing largely with the theory of the reaction mechanism of naphthalene (I) and divided into the following parts: 1) static fixation of the double bonds in I; 2) fusion of a 3rd ring to derivs. of I; 3) structure of the I nucleus and the manner in which it reacts; 4) anellation and excitation structures in the I series; 5) naphthalenoid and benzenoid bicyclic compds.; 6) manner in which quinoline

(II) and 1-hydroxyquinoline (III) react; 7) reactivity of aromatic polycyclic compds. (much of which involves the critical evaluation of previous work); and 8) an extensive exptl. part. The reactions of bicyclic compds. are discussed at length in terms of quantum-mech. calcns. of resonance energies (cf. Pauling and Wheland, C.A. 27, 3877; Sherman, C.A. 28, 6631.3; and Penney, C.A. 31, 2513.2). The hypothesis formulated by Marckwald (Ber. 23, 1015 (1890)) that the double bonds in I remain fixed loses its significance when anellation reactions (involving a 3rd ring) are considered. Previously the assumption was made that an "angular" tricyclic compound (IV) was normally formed. This was shown to be true in the case of 1-bromo- or 1-nitro-2-naphthylamine, either of which lose the 1-substituent on further cyclization to form the angular benzoquinoline. However, H. has shown that under certain conditions, a linear tricyclic form (V) may result. When 2 g. 1,2-MeC10H6NHAc (VI), m. 193°, was refluxed gently 5 hrs. with 2 g. arsenious acid, 7 g. glycerol, 7 g. H2SO4, and 5 g. AcOH, followed by treatment with 15 cc. H2O, digestion with NH4OH-CHCl3, filtration, evaporation of the CHCl3 extract, digestion with 8 g. Ac2O, saturation with NH4OH, reextn. with CHCl3, and treatment with 2 N HCl, H. obtained (after removal of residual VI, retreatment with NH4OH-CHCl3, and filtration through Al2O3) 0.53 g. 8-methyl-6,7-benzoquinoline (VII), b12 200°, m. 53-4° (not recrystd. due to high solubility in organic solvents); picrate, triclinic orange prisms (from MeOH), m. 212° (decomposition). The mother liquors gave no trace of the known "angular" 5,6-benzoquinoline (VIII) (picrate, m. 254°). The HCl salt (IX) of VII forms golden yellow needles. The yellow perchlorate and orange-red nitrate of VII contrast sharply with the corresponding colorless salts of VIII. In ultraviolet light, VII in Me2CO shows intense light blue, and IX a pale yellow fluorescence. On the other hand, VIII in organic solvents shows a very slight blue and its HCl salt gives a stronger blue fluorescence. 1,2-MeC10H6NHCOCH2Ac (cf. Limpach, C.A. 25, 3999), m. 135°, (0.25 g.) was shaken with 2.5 cc. concentrated H2SO4, allowed to stand 1 hr., poured into ice-H2O, made alkaline with NH4OH, extracted with CHCl3, evaporated, and taken up in MeOH, yielding 0.16 g. 2-hydroxy-4,8-dimethyl-6,7-benzoquinoline, pale yellow (sublimable) needles, m. 253°, insol. in aqueous alkaline solns. and in aqueous acids, but soluble in concentrated H2SO4 with a yellow color and yellowish green fluorescence, and giving a blue-green ultraviolet fluorescence in MeOH. On the other hand the "angular" 4-methyl-5,6-benzocarbostyril shows practically no ultraviolet fluorescence in MeOH and a deep violet fluorescence in H2SO4. Very similarly 0.35 g. 1,2-BrC10H6NHCOCH2Ac, m. 117°, in H2SO4 was cyclized to 0.225 g. 2-hydroxy-4-methyl-8-bromo-6,7-benzoquinoline, pale yellow needles, m. 232-4°. From 2 g. 1,2-MeC10H6NH2 and 1.6 g. AcCH2CO2Et, H. obtained 2.5 g. 1-MeC10H6NHCMe:CHCO2Et, m. 86-7° (from MeOH), 1.5 g. of which, gradually added to 20 g. paraffin oil at 270°, followed by heating 10 min. at 280°, gave 0.85 g. "linear" 2,8-dimethyl-4-hydroxy-6,7-benzoquinoline, yellow needles, m. 340° (decomposition) (after successive crystns. from C6H6, PhNO2, and EtOH), very soluble in 2 N NaOH, slightly soluble in hot 2 N HCl, showing marked blue-green ultraviolet fluorescence in NaOH, blue in NaOH, and yellowish green in concentrated H2SO4. From 0.3 g. 2-C10H7NHNH2.HCl in 4 cc. MeOH with 0.2 cc. cyclohexanone, H. obtained a nearly quant. yield of 5,6-benzo-1,2,3,4-tetrahydrocarbazole (X), m. 137° (from MeOH); dark brown picrate, m. 192° (from C6H6). The formation of X is expedited by adding 2 N HCl to the original reaction mixture 1,2-MeC10H6NHAc, m. 193°, was hydrolyzed with HCl in alc. and 3.5 g. of the resulting salt in 25 cc. 7 N HCl was treated at 0° in 8 cc. H2O with 1.34 g. NaNO2, followed by treatment with urea and addition to

12 g. $SnCl_2$ in 8 cc. HCl and 110 cc. H_2O, giving a nearly quant. yield of 1-methyl-2-hydrazinonaphthalene-HCl (XI), leaflets (from HCl), m. 195° (decomposition), converted by AcONa into the free base, m. 110° (from MeOH), reducing Fehling solution XI with Me_2CO gave 2,1-Me_2C:NNHC10H6Me, leaflets, m. 99°. By heating 0.85 g. XI in 2 cc. AcOH with 1 cc. cyclohexanone and 20 mg. $NiCl_2$ 2 hrs. at 180°, and then 3 hrs. at 200°, a small amount of X was obtained, showing that ring closure had removed the 1-Me group. Careful warming of 135g. 3,6-(H2N)(O2N)C6H3Me with 125 g. arsenic acid, 270 g. glycerol, and 250 g. H_2SO_4 about 6 hrs. gave 108 g. of a difficultly separated mixture of 6-nitro-7-methylquinoline (XII) and its 5-Me isomer (XIII), from which 11.4 g. XIII, m. 165° (colorless HCl salt), was separated by successive crystns. from MeOH and Me_2CO. Inasmuch as the components in the mother liquors from XIII could not be fractionally crystallized, the solution was evaporated, treated with 350 cc. MeOH, and shaken 40 min. with 180 cc. hot 20% KOH in MeOH, followed by the addition of 700 cc. MeOH, yielding a highly insol. conversion product of XIII, the filtrate and washings from which gave 54 g. pure XII, colorless needles (from EtOH), m. 140°; colorless HCl salt. $SnCl_2$ reduction of XIII yielded 6-amino-5-methylquinoline, coarse prisms, m. 163-4° (from C_6H_6) (yellow HCl salt; Ac derivative m. 168°), which when diazotized and poured into a Cu_2O suspension in EtOH gave 5-methylquinoline, pale yellow oil (picrate m. 213-14°) (cf. Skraup and Brunner, Monatsh. 7, 141(1886)), 0.43 g. of which after treatment 10 hrs. with 0.65 g. CrO_3 and 5 cc. 35% H_2SO_4 gave 5-carboxyquinoline, m. 330° (cf. Yakubovich, C.A.5,503). By a similar series of reactions XII gave the following: 6-amino-7-methylquinoline, plates, m. 139° (from C_6H_6); 7-methylquinoline (picrate, m. 235°, identical with that prepared from 3-$MeC_6H_4NH_2$ by the Skraup synthesis); 7-carboxyquinoline, m. 245°. XIII (1 g.) heated at the b.p. 3 min. with 12 cc. 10% KOH in MeOH gave 0.79 g. 1,2-bis(6-nitro-5-quinolyl)ethane, m. 300° (decomposition) (from AcOH), also formed when 2 N NaOH or alkaline arsenite solns. are used in place of KOH. The corresponding diamine, $C_{20}H_{18}N_4$, formed greenish yellow needles (from C_6H_6) (properties not given). By analogous procedures H. obtained from 6-nitro-5,8-dimethylquinoline 1,2-bis(6-nitro-8-methyl-5-quinolyl)ethane, nearly colorless needles, m. 257° (from pyridine or AcOH), and from 5-nitro-8-methylquinoline 1,2-bis(5-nitro-8-quinolyl)ethane, needles, m. 221° (from C_6H_6 or AcOH), which on further treatment with alkali gave a deep violet color (cf. Trautmann, Ber. 23, 3673(1890)). 2-$O_2NC_6H_4Me$ in cooled absolute Et_2O, treated with an equimol. amount of alc.-free EtOK in Et_2O, the mixture let stand overnight, shaken with H_2O, and the Et_2O layer dried, filtered through Al_2O_3, and concentrated, gave 25-30% o,o'-dinitrobibenzyl, needles (from MeOH), m. 122°. Knuppel's reaction (cf. Ann. 310, 75(1900)), in which 6-nitroquinoline was heated with MeONa, gave 80% of a quinazone N-oxide (XIV), yellow needles, decomposing 330° (from AcOH) (red HCl salt (from H_2O)), which when distilled with Fe powder gave the O-free quinazone, $C_{18}H_{10}N_4$, pale yellow leaflets (from C_6H_6), m. 369°, sublimes undecompd. at 400°, gives a colorless HCl solution, and when heated with Zn dust, yields a bluish green semiquinone-like compound that may be reoxidized to the original quinazone by $KMnO_4$. A reaction analogous to that giving XIV yielded from XII the 7,7'-di-Me derivative, yellow needles (from AcOH), m. 355° (decomposition), yielding, on reduction, the dimethylquinazone, $C_{20}H_{14}N_4$, long, pale yellow needles, m. 380° (from xylene). Similarly 6-nitro-7,8-dimethylquinoline gave the corresponding tetra-Me derivative of XIV, yellowish green needles (from $PhNO_2$), decomposing above 330° and forming, when distilled with Fe, the tetramethylquinazone, pale yellow needles, m. 354°.

6-Nitroquinoline (1 g.), 0.5 g. KCN, 15 cc. EtOH, 3 cc. H_2O, and 0.5 g.

KOH heated 4 hrs. gave 0.5 g. 5-cyano-6-ethoxyquinoline, needles, m. 130° (from MeOH), very resistant to HNO_2, hot concentrated HCl, and cold H_2SO_4, whose colorless HCl and H_2SO_4 salts are difficultly soluble in H_2O. By a similar reaction, using MeOH in place of EtOH, 5-cyano-6-methoxyquinoline, needles (from MeOH), m. 179°, was obtained. To a cooled mixture of 5 g. 6-nitroquinoline, 6 g. $HONH_2.HCl$, and 90 cc. EtOH was added (in 1 portion) 30 cc. 20% KOH in MeOH. The exothermic reaction gave rise to 94% 5-amino-6-nitroquinoline (XV), yellow needles, m. 272° (yellow, difficultly soluble HCl salt), which with $SnCl_2$ in HCl gave 5,6-diaminoquinoline chlorostannate; the latter, after detinning with H_2S, yielded the HCl salt, pale yellow crystals, 0.1 g. of which when heated with 0.12 g. benzil in 5 cc. alc. and small amts. of AcONa gave the substituted quinoxaline, $C_{23}H_{15}N_3$ (0.88 g.), plates from C_6H_6, m. 205°; the di-Ac derivative m. 252° with decomposition to form 5,6-(methylimidazolo)quinoline, m. 200° (hydrate, m. 70°). The latter was more readily prepared by heating 0.5 g. XV in 5 cc. AcOH several hrs. with 2.1 g. $SnCl_2$ in 4 cc. HCl, followed by detinning, evaporation, treatment with NH_4OH, and extraction with Me_2CO. Similarly, when XV was reduced in the presence of HCO_2H (instead of AcOH), 5,6-imidazoloquinoline, m. 214° (from C_6H_6) (hydrate, m. 78°), was formed. By diazotization, the NH_2 group in XV was replaced by iodine (using KI and Cu-bronze), yielding a resin which after trituration with HCl, extraction with $NH_4OHCHCl_3$, followed by washing with aqueous Na_2SO_4 and H_2O, and passing the $CHCl_3$ solution through Al_2O_3, gave red needles, which on repeated crystallization from MeOH and C_6H_6 yielded colorless 5-iodo-6-chloroquinoline, m. 136°. Deiodination with Cu-bronze in boiling $PhNO_2$ gave 6,6'-dichloro-5,5'-biquinoline, colorless polyhedrons, m. 205°. When, however, the iodine was removed by means of HI in AcOH, 5-iodo-6-chloroquinoline gave 6-chloroquinoline, m. 40-1°. Skraub's cyclization of 0.5 g. 5-nitro-6-aminoquinoline (Kaufmann and Zeller, C.A. 12, 1390), using arsenic acid gave 0.115 g. 4,7-phenanthroline, polyhedrons (from C_6H_6), m. 174° (showing only a faint ultraviolet fluorescence), also obtained (in 65% yield) by cyclization of 5-bromo-6-aminoquinoline. Evidently NO_2 or Br in position 5 fails to block the formation of 4,7-phenanthroline. On the other hand, when 1 g. 6-acetamido-5-methylquinoline was heated gently 10-12 hrs. with 0.9 g. arsenic acid, 6 g. glycerol, 6 g. H_2SO_4, and 5 g. glacial AcOH, followed successively by treatment with H_2O, extraction with NH_4OH-$CHCl_3$, extraction with 2 N HCl, reextn. with NH_4OH-$CHCl_3$, evaporation, treatment of the dry extract with 3 cc. pyridine and 0.2 g. $4\text{-}MeC_6H_4SO_2Cl$ (to remove any unchanged starting product), and continued purification by extracting alternately with alkaline $CHCl_3$ and HCl, filtering the $CHCl_3$ solution through Al_2O_3, and finally subjecting the product to microdistn., using a water pump, H. obtained 3 fractions: (a) subliming 180°, (b) yellow oil, b. 200-20°, and (c) a red oil, b. 235°. Of these (b) gave 12 mg. linear 10-methyl-1,5-anthrazoline hydrate, $C_{15}H_{10}N_2.3H_2O$, felted needles, m. 62°, giving a yellow solution in acids and showing a brilliant bluish violet (ultraviolet) fluorescence. 8-Methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline (XVI), m. 225-6° (from EtOH), was prepared in 70% yield by heating 0.5 g. 6-hydrazino-8-methylquinoline (the synthesis of which is not given) with 3 cc. AcOH and 1.5 cc. cyclohexanone 6 hrs. and purifying the product by methods similar to those given above. XVI was also readily obtained in 75% yield by heating 0.33 g. of the substituted cyclohexanone hydrazone (XVII), m. 189°, at 200-240° with 15 mg. dry $NiCl_2$, or (in only 34% yield) by heating this same hydrazone with 2 N H_2SO_4. The following steps also led to the formation of XVI:

4-nitro-2,5-xylidine → Skraup's synthesis 50% 6-nitro-5,8-dimethylquinoline, m. 118° (from alc.) → $SnCl_2$ 6-amino derivative, b12 194°, prisms, m. 175° → HCl salt, yellow → 7 N HCl+HNO_2 diazo derivative → $SnCl_2$ chlorostannate → H_2S+HCl 85% 6-hydrazino-5,8-dimethylquinoline-HCl, yellow needles (free base (XVIII), m. 185°) → cyclohexanone 30% XVI. The ultraviolet absorption spectra of XVI prepared by the various methods were identical and showed a striking similarity to that of 7,8-dimethyl-10,11-tetramethylene-5,6(N)-pyrroquinoline. XVIII fails to undergo cyclization to XVI unless HCl is present. 6-Hydrazino-8-methylquinoline-HCl and MeCOEt in AcOH gave 40% 8,10,11-trimethyl-5,6(N)-pyrroquinoline, m. 188° (from EtOH), also formed in poor yield from the HCl salt of XVIII with concomitant removal of a Me group. Similarly, 0.5 g. 5-hydrazinoquinoline-HCl and cyclohexanone in AcOH gave 0.42 g. 10,11-tetramethylene-5(N),6-pyrroquinoline (XIX), m. 289° (from Me_2CO). XIX was also isolated in 1-2% yield after extensive purification from 5-hydrazino-6-methylquinoline, m. 158° (pale yellow HCl salt).

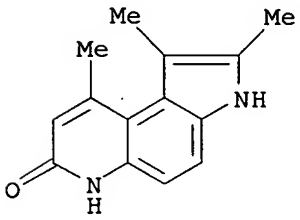
$SnCl_2$ reduction of 15 g. 6-nitro-2-hydroxylepidine gave 9.6 g. 2-hydroxy-4-methyl-6-aminoquinoline (XX), pale yellow, m. above 300°, cyclizing in the presence of arsenic acid, glycerol, and H_2SO_4-AcOH, followed by successive treatments with HCl and NH_4OH, to form 2-hydroxy-4-methyl-4,7-phenanthroline (XXI), colorless prisms, the "angularity" of which was attested to by its very faint ultraviolet fluorescence, its ready solubility in aqueous NaOH and in boiling aqueous Na_2CO_3, and by the fact that its salts are colorless. 2,5-Xylidine, when heated at 160° with an equimol. amount of $AcCH_2CO_2Et$, gave the N-acetylacetyl derivative, m. 96° (from aqueous MeOH), which when heated 0.5 hr. on a steam bath with 6 parts concentrated H_2SO_4 gave (after pouring on ice) 90% 2-hydroxy-4,5,8-trimethylquinoline, m. 238° (from EtOH); 6-nitro derivative, pale yellow, m. 275° (from AcOH or EtOH); 6-amino derivative (XXII) (formed from the orange-red Sn double salt), pale yellow leaflets, m. 302° (from aqueous NH_4OH or EtOH) (colorless HCl salt, difficultly soluble in H_2O). The Skraup cyclization of XXII gave 2-hydroxy-4,9,10-trimethyl-1,5-anthrazoline (XXIII), pale yellow needles (from glacial AcOH or Ac_2O), m. 290°, whose linear structure was indicated by the yellow color of its acid solns., its insoly. in alkali, and its strong blue ultraviolet fluorescence in MeOH. On diazotization, followed by $SnCl_2$ reduction, XX gave 90% 2-hydroxy-4-methyl-6-hydrazinoquinoline, colorless needles from H_2O, decomposing 240°, reducing Fehling solution in the cold, and forming a colorless HCl salt, which, when cyclized in the presence of MeCOEt and glacial AcOH, gave 90% 2-hydroxy-4,10,11-trimethyl-5,6(N)-pyrroquinoline, needles (from alc.), m. above 300° (decomposition); yellow HCl salt. When an analogous cyclization was carried out in the presence of cyclohexanone, 2-hydroxy-4-methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline, m. above 300°, was formed; golden yellow HCl salt. Diazotization of XXII, followed by reduction, gave the yellow chlorostannate of 2-hydroxy-4,5,8-trimethyl-6-hydrazinoquinoline, which in hot H_2O, followed by filtration of the stannic acid, reacted with MeCOEt to form the corresponding substituted hydrazone, pale yellow needles, m. 112° (from a buffered AcONa solution), which failed to cyclize when treated with $ZnCl_2$ at 200-60°, giving only 4,5,8-trimethylcarbostyril, m. 236°. Other attempts to cyclize the compound were equally unsuccessful. 2,3-Diphenyl-4,5-benzoindole, colorless prisms with blue-green iridescence, m. 166-7°, (3 g.) was formed from 1 g. 2-$H_2NC_{10}H_7$, 0.5 g. $C_{10}H_7NH_2$.HCl, and 2.2 g. benzoin at 140-65° (cf. Japp and Murray, J. Chemical Society 65, 889(1894)). 2,1-$H_2NC_{10}H_6Me$ subjected to a similar reaction gave 1-methyl-2-desylaminonaphthalene, 2,1-[PhC(OH):CPhNH]$C_{10}H_6Me$, pale yellow, m. 152-3° (from $CHCl_3$-MeOH),

which could not be cyclized by the use of ZnCl2, H2SO4, H3PO4, SnCl4, NiCl2, or SOCl2. The structure of this compound was shown by HClMeOH hydrolysis to benzoin and 2,1-H2NC10H6Me. The resonance energy of I was calculated from the total hydrogenation to decahydronaphthalene and also from its partial hydrogenation to tetrahydronaphthalene. The values obtained were, resp., 63.5 and 63.1 kcal./mol. and the approx. resonance energy per ring was 31.5 kcal. (cf. also Pauling, "Nature of the Chemical Bond," C.A. 33, 6700.4).

IT **86269-88-7**, 3H-Pyrrolo[3,2-f]quinolin-7-ol, 1,2,9-trimethyl-
(preparation of)

RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)



10080926

=> d his

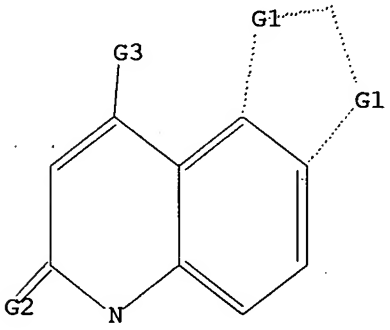
(FILE 'HOME' ENTERED AT 16:05:03 ON 12 APR 2005)

FILE 'REGISTRY' ENTERED AT 16:05:13 ON 12 APR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 71 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:06:04 ON 12 APR 2005
L4 5 S L3

FILE 'CAOLD' ENTERED AT 16:06:51 ON 12 APR 2005
L5 0 S L3

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,N

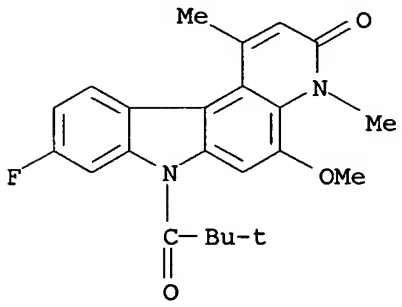
G2 O,S,N

G3 C,O,S,N,X

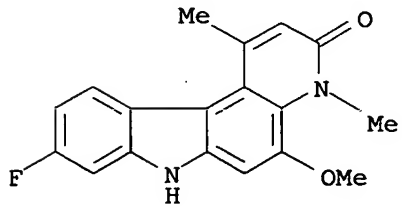
10080926

=> d bib abs hitstr 1-5

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:39690 CAPLUS
DN 142:240350
TI An efficient procedure for the deprotection of N-pivaloylindoles, carbazoles and β-carbolines with LDA
AU Avendano, Carmen; Sanchez, J. Domingo; Menendez, J. Carlos
CS Departamento de Quimica Organica, Farmaceutica, Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain
SO Synlett (2005), (1), 107-110
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English
AB Treatment of variously substituted indoles with an excess of LDA at 40-45 °C led to their fast and efficient deprotection. This method was also extended to N-pivaloylcarbazoles and β-carbolines.
IT **845619-80-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indoles, carbazoles, and β-carboline via LDA-mediated deprotection of N-pivaloylindoles, -carbazoles, or -β-carboline)
RN 845619-80-9 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 7-(2,2-dimethyl-1-oxopropyl)-9-fluoro-4,7-dihydro-5-methoxy-1,4-dimethyl- (9CI) (CA INDEX NAME)



IT **845619-82-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indoles, carbazoles, and β-carboline via LDA-mediated deprotection of N-pivaloylindoles, -carbazoles, or -β-carboline)
RN 845619-82-1 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 9-fluoro-4,7-dihydro-5-methoxy-1,4-dimethyl- (9CI) (CA INDEX NAME)



10080926

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:658121 CAPLUS
DN 137:201294
TI Preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compounds as androgen receptor modulators
IN Zhi, Lin; Van Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Higuchi, Robert I.
PA Ligand Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002066475	A2	20020829	WO 2002-IB537	20020223
	WO 2002066475	A3	20030123		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2002183346	A1	20021205	US 2002-80926	20020222
	CA 2434299	AA	20020829	CA 2002-2434299	20020223
	EP 1363909	A2	20031126	EP 2002-702589	20020223
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2002007549	A	20040803	BR 2002-7549	20020223
	JP 2004524309	T2	20040812	JP 2002-565989	20020223
PRAI	US 2001-271189P	P	20010223		
	WO 2002-IB537	W	20020223		

OS MARPAT 137:201294
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title nonsteroidal tricyclic compds. I-VIII [wherein R1 = H, halo, NO2, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl or heteroalkyl; R2 = H, halo, Me, CF3, CHF2, CH2F, CF2Cl, CN, CF2OR12, CH2OR12, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, or alkynyl; R3-R8 = independently H, halo, OR12, NR12R13, SO0-2R12, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, (hetero)aryl, or arylalkyl; or R3R5 or R5R7 = a bond; or C2R4R6 or C2R6R8 = (un)substituted carbocyclic or heterocyclic ring; R9 and R10 = independently H, halo, CN, OR12, NR12R13, Cm(R12)2mOR13, SO0-2R12, NR12COR13, or (un)substituted (halo)alkyl, heteroalkyl, or arylalkyl; R11 = H, halo, CN, OR14, NR14R15, SO0-2R14, CH2R14, COR14, CO2R14, CONR13R14, or (un)substituted (halo)alkyl or heteroalkyl; R12 and R13 = independently H or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, or (hetero)aryl; R14 = H, COR15, CO2R15, CONR15R16, or (un)substituted

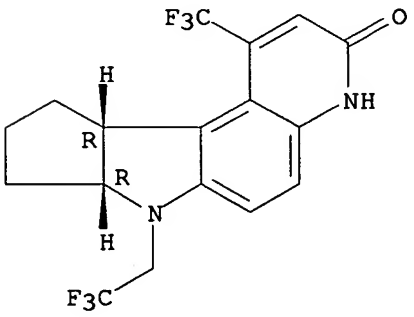
(halo)alkyl, heteroalkyl, or (hetero)aryl; R15 and R16 = independently H or (un)substituted (halo)alkyl, or heteroalkyl; W = O or S; X = O, S, or NR14; Y = O, S, NR12, NOR12, or CR12R13; Z = O, S, or NR12; n = 0-2; m = 0-2; or pharmaceutically acceptable salts thereof] were prepared as modulators of androgen receptors. For example, cyclization of 6-hydrazino-4-trifluoromethylquinolin-2(1H)-one with 3-pentanone afforded the cis-5,6-dihydro-7H-pyrrolo[3,2-f]quinolin-2(1H)-one. Oxidation with DDQ in CH2Cl2 gave 6-ethyl-5-methyl-7-(2,2,2-trifluoroethyl)-4-trifluoromethyl-1H-pyrrolo[3,2-f]quinolin-2(1H)-one (IX). The latter exhibited 76% androgen receptor agonist efficacy with a potency (EC50) of 7.6 nM relative to dihydrotestosterone in co-transfection assays using CV-1 cells and displayed androgen receptor binding activity (IC50) of 1.7 nM. Pharmaceutical compns. and formulations of IX are also disclosed. I-VIII are useful for the treatment of acne, male-pattern baldness, impotence, sexual dysfunction, wasting disease, hirsutism, hypogonadism, prostatic hyperplasia, osteoporosis, cancer cachexia, and hormone-dependent cancers (no data). Pharmaceutical compns. and formulations of IX are also disclosed.

IT **453592-26-2P**
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-26-2 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

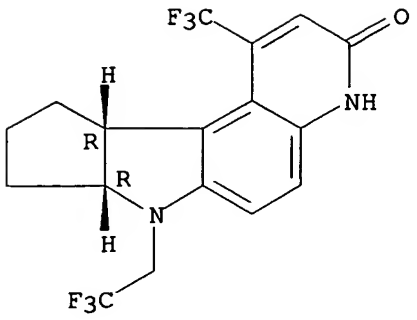


IT **453592-85-3P 453592-86-4P**
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-85-3 CAPLUS

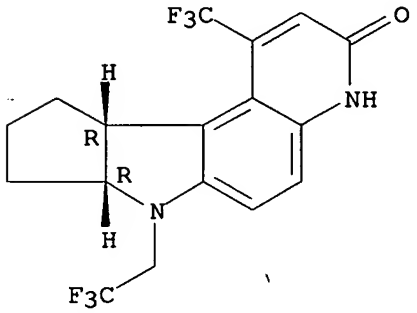
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

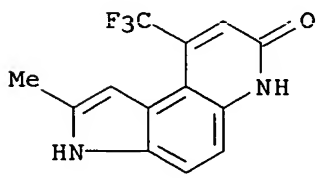


RN 453592-86-4 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(-)- (9CI) (CA INDEX NAME)

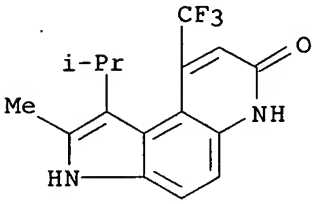
Rotation (-). Absolute stereochemistry unknown.



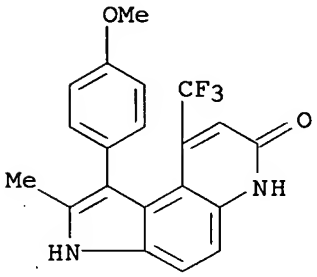
IT **453592-19-3P 453592-20-6P 453592-22-8P**
453592-24-0P 453592-25-1P 453592-30-8P
453592-39-7P 453592-41-1P 453592-46-6P
453592-47-7P 453592-52-4P 453592-53-5P
453592-54-6P 453592-57-9P 453592-60-4P
453592-71-7P 453592-72-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)
RN 453592-19-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-(9CI) (CA INDEX NAME)



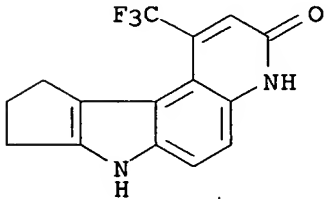
RN 453592-20-6 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(1-methylethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



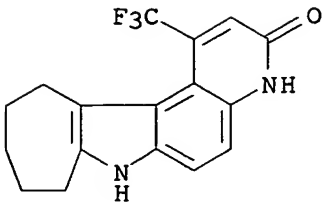
RN 453592-22-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-24-0 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)

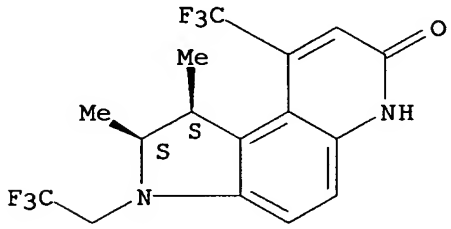


RN 453592-25-1 CAPLUS
CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10,11,12-hexahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



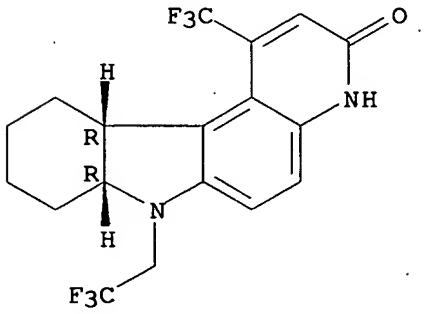
RN 453592-30-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



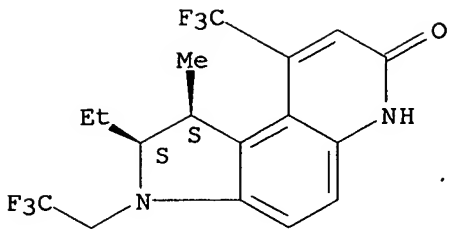
RN 453592-39-7 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7,7a,8,9,10,11,11a-octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,11aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



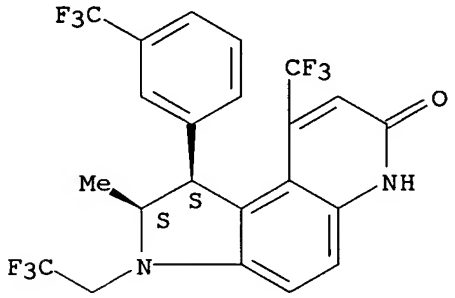
RN 453592-41-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-1,2,3,6-tetrahydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



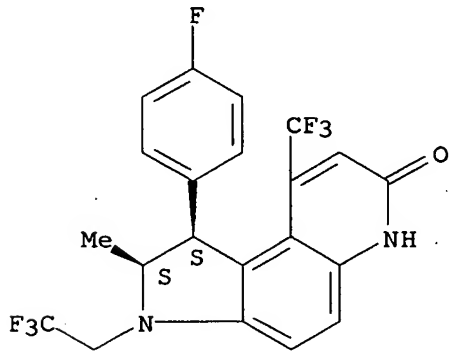
RN 453592-46-6 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

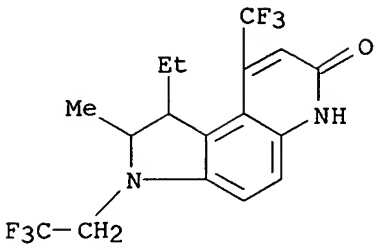


RN 453592-47-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

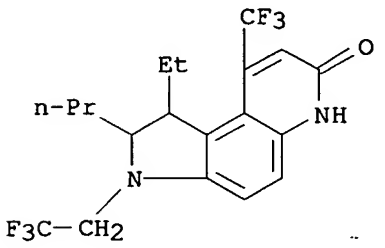
Relative stereochemistry.



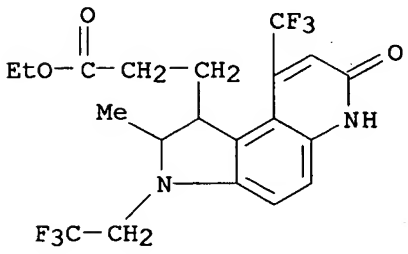
RN 453592-52-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



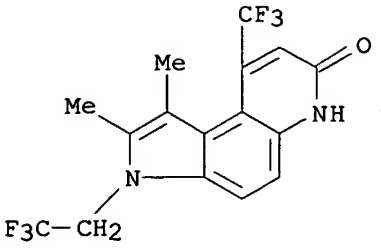
RN 453592-53-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



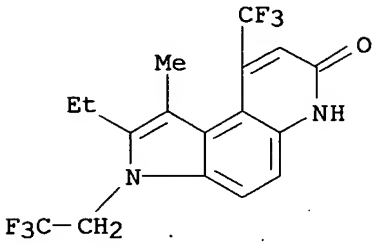
RN 453592-54-6 CAPLUS
CN 1H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 2,3,6,7-tetrahydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



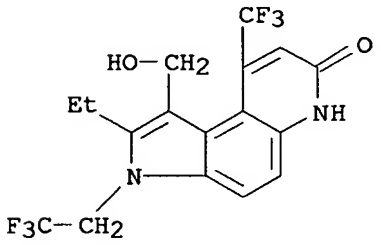
RN 453592-57-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



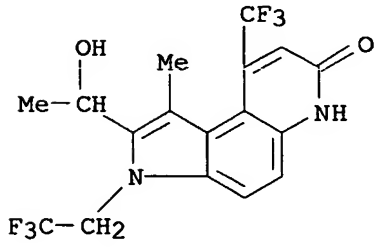
RN 453592-60-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-71-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-(hydroxymethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

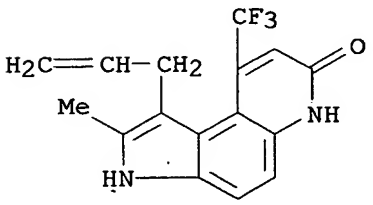


RN 453592-72-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-hydroxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

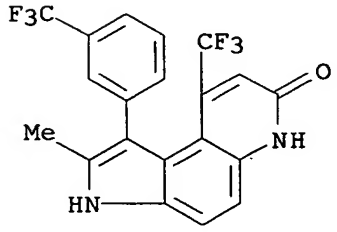


IT **453592-21-7P 453592-23-9P 453592-28-4P**
453592-32-0P 453592-33-1P 453592-34-2P
453592-35-3P 453592-36-4P 453592-37-5P
453592-38-6P 453592-40-0P 453592-42-2P
453592-43-3P 453592-44-4P 453592-45-5P
453592-48-8P 453592-49-9P 453592-50-2P
453592-51-3P 453592-59-1P 453592-61-5P
453592-62-6P 453592-63-7P 453592-64-8P
453592-65-9P 453592-67-1P 453592-68-2P
453592-69-3P 453592-73-9P 453592-74-0P
453592-75-1P 453592-77-3P 453592-78-4P
453592-79-5P 453592-80-8P 453592-82-0P
453592-83-1P 453592-84-2P 453593-25-4P
453593-26-5P 453593-30-1P 453593-31-2P
453593-32-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-21-7 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

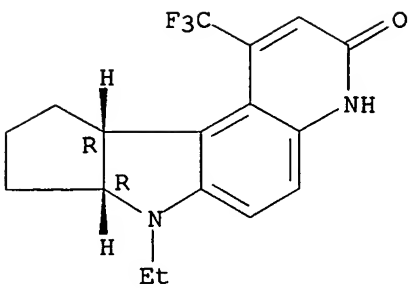


RN 453592-23-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



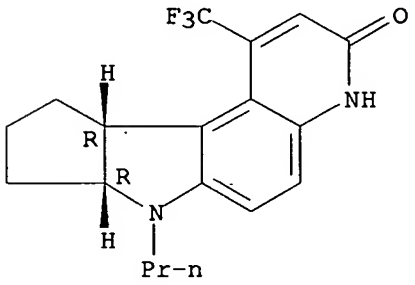
RN 453592-28-4 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-ethyl-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



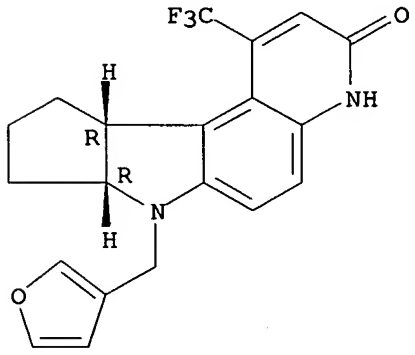
RN 453592-32-0 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-propyl-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



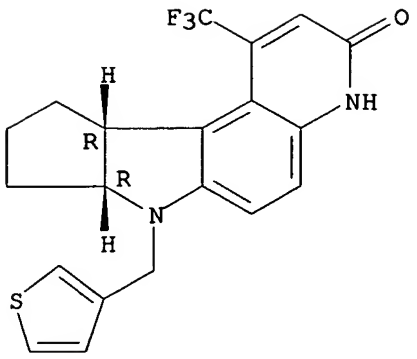
RN 453592-33-1 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(3-furanylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



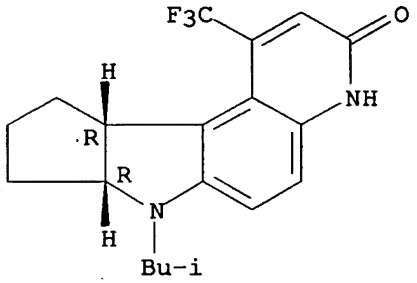
RN 453592-34-2 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(3-thienylmethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



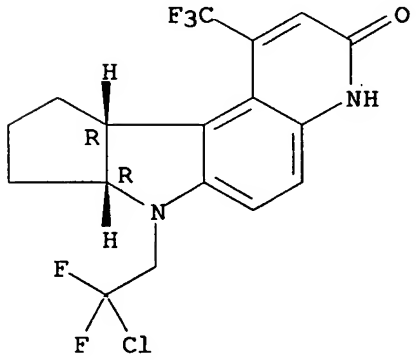
RN 453592-35-3 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2-methylpropyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 453592-36-4 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2-chloro-2,2-difluoroethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

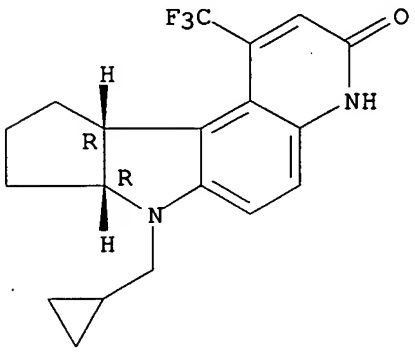
Relative stereochemistry.



RN 453592-37-5 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(cyclopropylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

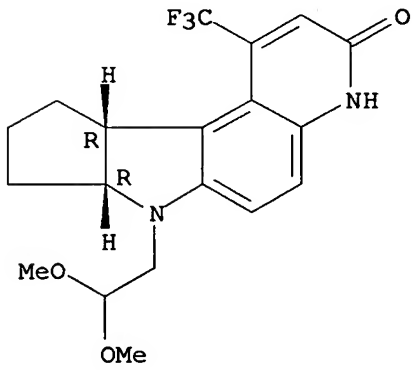
Relative stereochemistry.



RN 453592-38-6 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2,2-dimethoxyethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

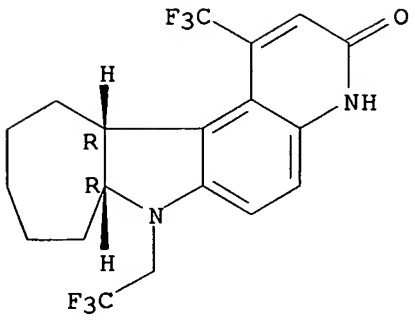
Relative stereochemistry.



RN 453592-40-0 CAPLUS

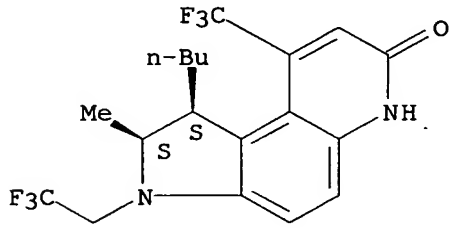
CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,11,12,12a-octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,12aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



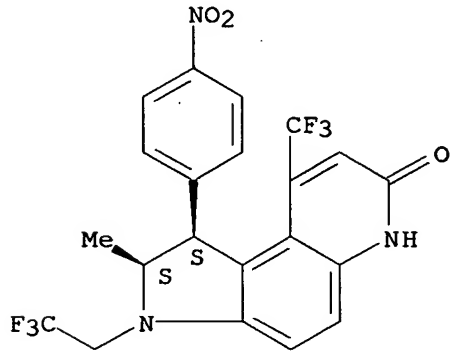
RN 453592-42-2 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-butyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



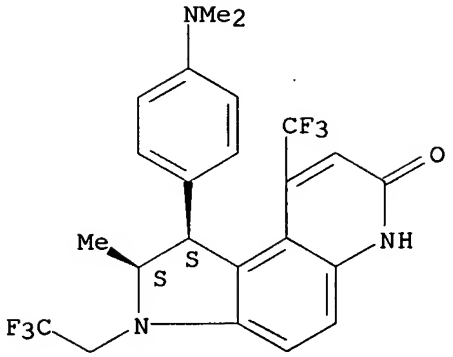
RN 453592-43-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(4-nitrophenyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



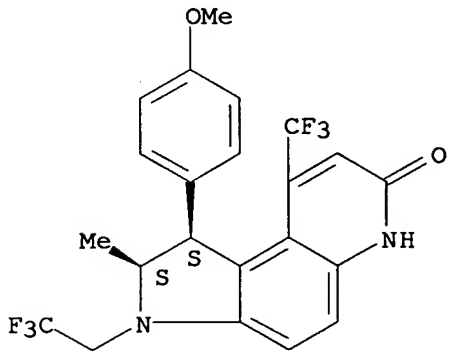
RN 453592-44-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[4-(dimethylamino)phenyl]-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

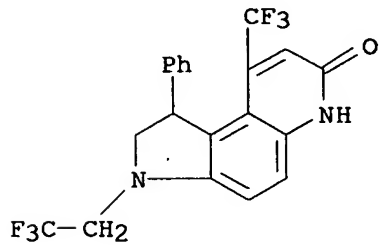


RN 453592-45-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

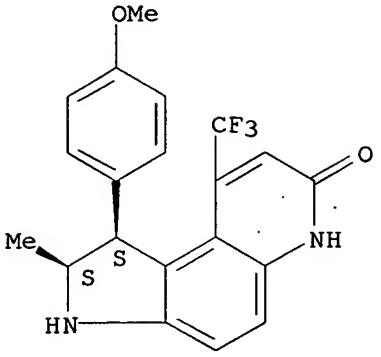


RN 453592-48-8 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-phenyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



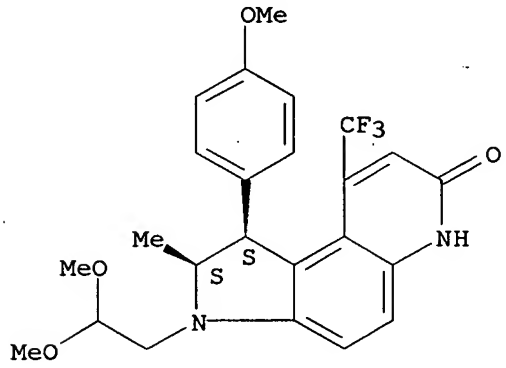
RN 453592-49-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



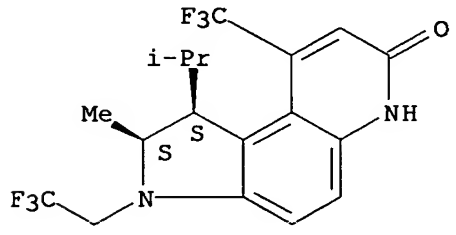
RN 453592-50-2 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-dimethoxyethyl)-1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

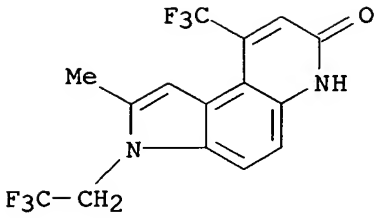


RN 453592-51-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(1-methylethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

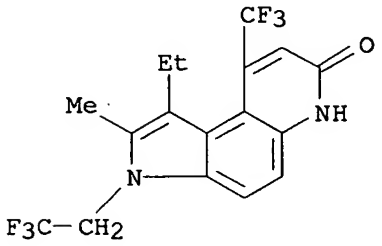
Relative stereochemistry.



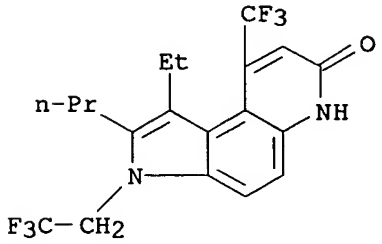
RN 453592-59-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



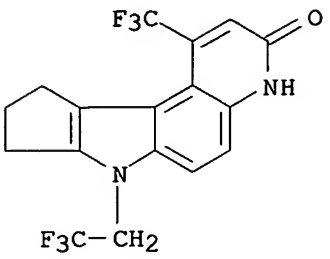
RN 453592-61-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



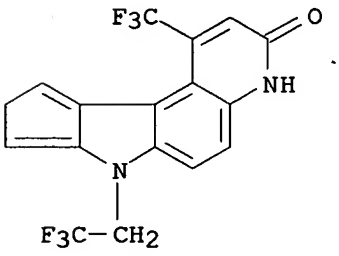
RN 453592-62-6 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



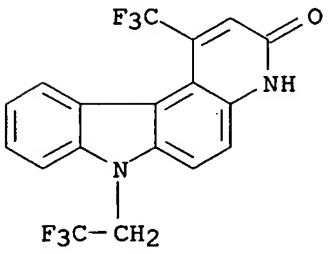
RN 453592-63-7 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



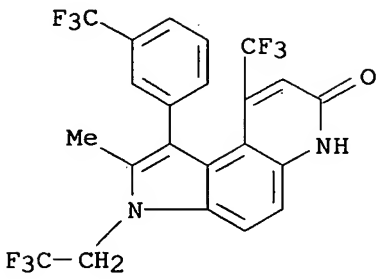
RN 453592-64-8 CAPLUS
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,9-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



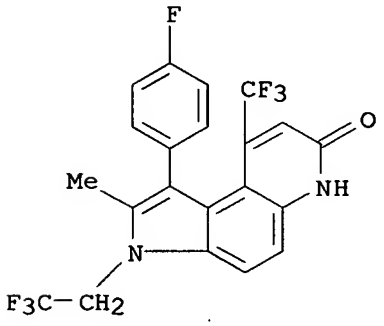
RN 453592-65-9 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



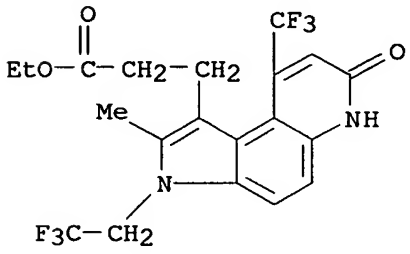
RN 453592-67-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



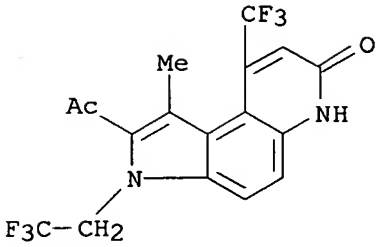
RN 453592-68-2 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



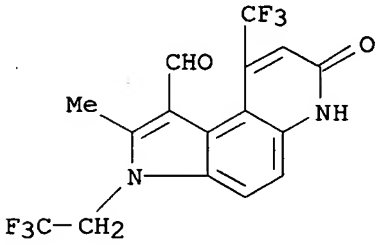
RN 453592-69-3 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



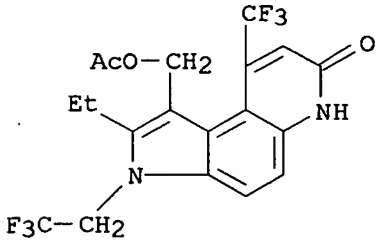
RN 453592-73-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-acetyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



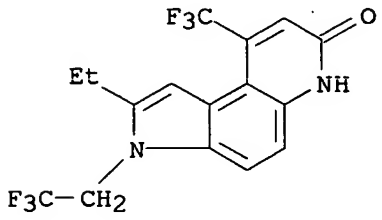
RN 453592-74-0 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-1-carboxaldehyde, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



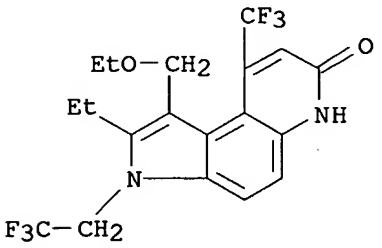
RN 453592-75-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[(acetyloxy)methyl]-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



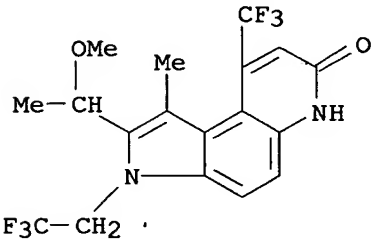
RN 453592-77-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



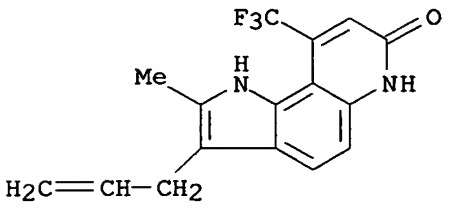
RN 453592-78-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(ethoxymethyl)-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



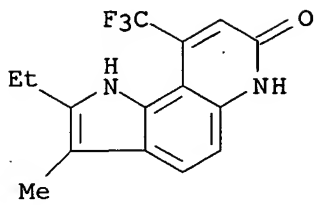
RN 453592-79-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-methoxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



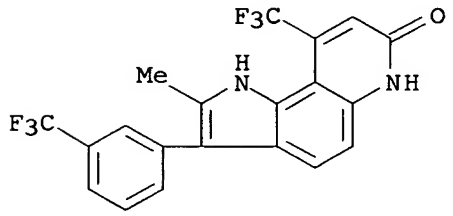
RN 453592-80-8 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-3-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



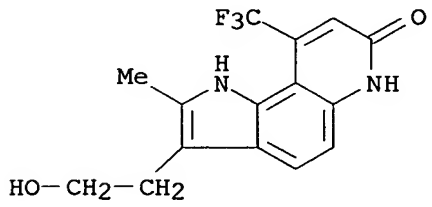
RN 453592-82-0 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 2-ethyl-1,6-dihydro-3-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



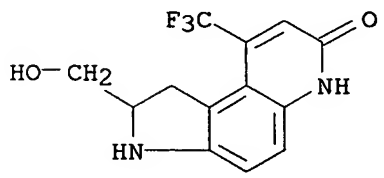
RN 453592-83-1 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-9-(trifluoromethyl)-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



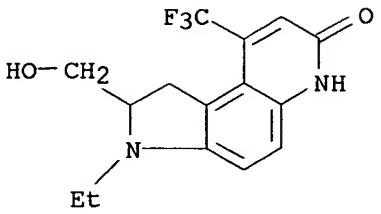
RN 453592-84-2 CAPLUS
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-3-(2-hydroxyethyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



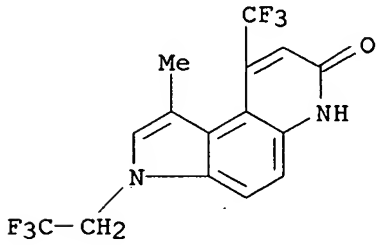
RN 453593-25-4 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



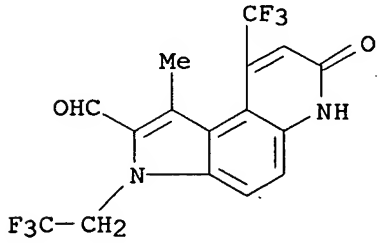
RN 453593-26-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-ethyl-1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



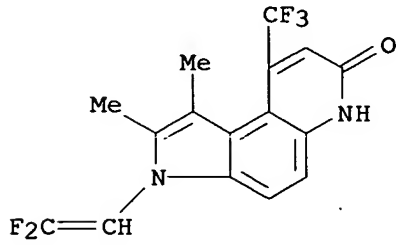
RN 453593-30-1 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



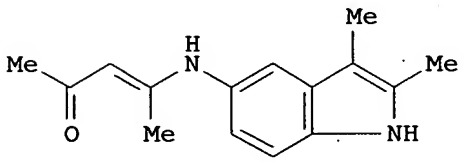
RN 453593-31-2 CAPLUS
CN 3H-Pyrrolo[3,2-f]quinoline-2-carboxaldehyde, 6,7-dihydro-1-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-32-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-difluoroethenyl)-3,6-dihydro-1,2-dimethyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:455695 CAPLUS
DN 131:213835
TI Reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines
AU Yamashkin, S. A.; Trushkov, I. V.; Tomilin, O. B.; Terekhin, I. I.; Yurovskaya, M. A.
CS Mordovian State Pedagogical Institute, Sarinsk, 430007, Russia
SO Chemistry of Heterocyclic Compounds (New York)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9), 1050-1065
CODEN: CHCCAL; ISSN: 0009-3122
PB Consultants Bureau
DT Journal
LA English
GI

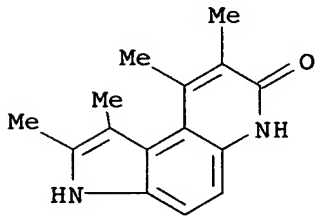


I

AB The concept of regioorientation is proposed for the annelation of the pyridine ring with the participation of 5-, 6-, and 7-aminoindoles (e.g. ,I). The conclusions based on the exptl. data are supported by semiempirical AM1, PM3, and MNDO quantum-chemical calcns.

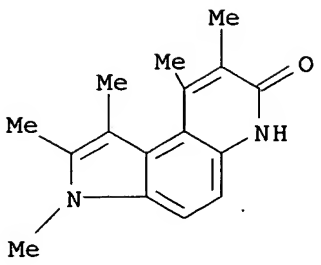
IT **243669-00-3 243669-02-5 243669-06-9**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines)

RN 243669-00-3 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,8,9-tetramethyl- (9CI) (CA INDEX NAME)

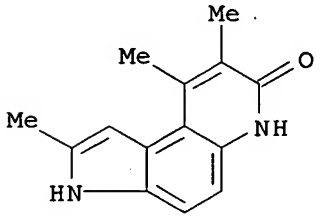


RN 243669-02-5 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,3,8,9-pentamethyl- (9CI) (CA INDEX NAME)

10080926

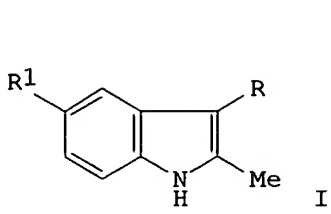


RN 243669-06-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2,8,9-trimethyl- (9CI) (CA INDEX NAME)

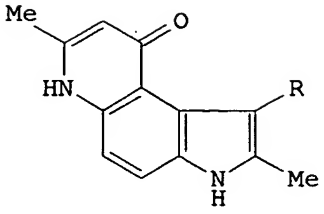


RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

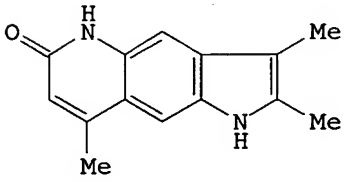
L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:438395 CAPLUS
DN 99:38395
TI Synthesis of pyrroloquinolones
AU Yamashkin, S. A.; Yudin, L. G.; Kost, A. N.
CS Mosk. Gos. Univ., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1983), (4), 493-7
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 99:38395
GI



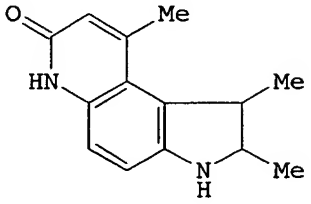
I



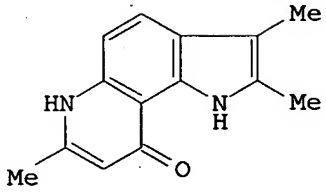
II



III



IV



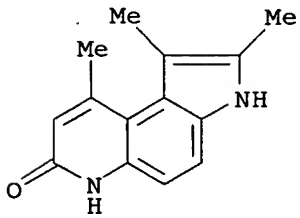
V

AB Intramol. cyclocondensation of I (R = Me, H; R1 = EtO2CCH:CMeNH) by refluxing in biphenyl gave 89 and 95% pyrroloquinolines II. Similarly, refluxing I (R = Me, R1 = MeCOCH2CONH) in F3CCO2H gave a mixture containing III and IV. Refluxing I (R = Me, R1 = EtO2CCH:CMeNH in the 6 position) with biphenyl gave 90% V.

IT **86269-88-7P 86269-91-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

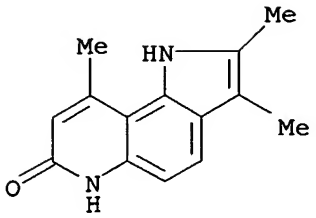
RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)



RN 86269-91-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2,3,9-trimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1948:32006 CAPLUS
DN 42:32006
OREF 42:6783h-i,6784a-i,6785a-i,6786a-i,6787a-i,6788a-e
TI Orienting experiments on the reaction mechanism of aromatic bicyclic compounds
AU Huisgen, Rolf
CS Univ. Munich, Weilheim, Germany
SO Ann. (1948), 559, 101-52
DT Journal
LA Unavailable
OS CASREACT 42:32006
GI For diagram(s), see printed CA Issue.
AB A comprehensive monograph dealing largely with the theory of the reaction mechanism of naphthalene (I) and divided into the following parts: 1) static fixation of the double bonds in I; 2) fusion of a 3rd ring to derivs. of I; 3) structure of the I nucleus and the manner in which it reacts; 4) anellation and excitation structures in the I series; 5) naphthalenoid and benzenoid bicyclic compds.; 6) manner in which quinoline (II) and 1-hydroxyquinoline (III) react; 7) reactivity of aromatic polycyclic compds. (much of which involves the critical evaluation of previous work); and 8) an extensive exptl. part. The reactions of bicyclic compds. are discussed at length in terms of quantum-mech. calcns. of resonance energies (cf. Pauling and Wheland, C.A. 27, 3877; Sherman, C.A. 28, 6631.3; and Penney, C.A. 31, 2513.2). The hypothesis formulated by Marckwald (Ber. 23, 1015 (1890)) that the double bonds in I remain fixed loses its significance when anellation reactions (involving a 3rd ring) are considered. Previously the assumption was made that an "angular" tricyclic compound (IV) was normally formed. This was shown to be true in the case of 1-bromo- or 1-nitro-2-naphthylamine, either of which lose the 1-substituent on further cyclization to form the angular benzoquinoline. However, H. has shown that under certain conditions, a linear tricyclic form (V) may result. When 2 g. 1,2-MeC10H6NHAc (VI), m. 193°, was refluxed gently 5 hrs. with 2 g. arsenious acid, 7 g. glycerol, 7 g. H2SO4, and 5 g. AcOH, followed by treatment with 15 cc. H2O, digestion with NH4OH-CHCl3, filtration, evaporation of the CHCl3 extract, digestion with 8 g. Ac2O, saturation with NH4OH, reextn. with CHCl3, and treatment with 2 N HCl, H. obtained (after removal of residual VI, retreatment with NH4OH-CHCl3, and filtration through Al2O3) 0.53 g. 8-methyl-6,7-benzoquinoline (VII), b12 200°, m. 53-4° (not recrystd. due to high solubility in organic solvents); picrate, triclinic orange prisms (from MeOH), m. 212° (decomposition). The mother liquors gave no trace of the known "angular" 5,6-benzoquinoline (VIII) (picrate, m. 254°). The HCl salt (IX) of VII forms golden yellow needles. The yellow perchlorate and orange-red nitrate of VII contrast sharply with the corresponding colorless salts of VIII. In ultraviolet light, VII in Me2CO shows intense light blue, and IX a pale yellow fluorescence. On the other

hand, VIII in organic solvents shows a very slight blue and its HCl salt gives a stronger blue fluorescence. 1,2-MeC10H6NHCOCH2Ac (cf. Limpach, C.A. 25, 3999), m. 135°, (0.25 g.) was shaken with 2.5 cc. concentrated H2SO4, allowed to stand 1 hr., poured into ice-H2O, made alkaline with NH4OH, extracted with CHCl3, evaporated, and taken up in MeOH, yielding 0.16 g. 2-hydroxy-4,8-dimethyl-6,7-benzoquinoline, pale yellow (sublimable) needles, m. 253°, insol. in aqueous alkaline solns. and in aqueous acids, but soluble in concentrated H2SO4 with a yellow color and yellowish green fluorescence,

and giving a blue-green ultraviolet fluorescence in MeOH. On the other hand the "angular" 4-methyl-5,6-benzocarbostyril shows practically no ultraviolet fluorescence in MeOH and a deep violet fluorescence in H2SO4. Very similarly 0.35 g. 1,2-BrC10H6NHCOCH2Ac, m. 117°, in H2SO4 was cyclized to 0.225 g. 2-hydroxy-4-methyl-8-bromo-6,7-benzoquinoline, pale yellow needles, m. 232-4°. From 2 g. 1,2-MeC10H6NH2 and 1.6 g. AcCH2CO2Et, H. obtained 2.5 g. 1-MeC10H6NHCMe:CHCO2Et, m. 86-7° (from MeOH), 1.5 g. of which, gradually added to 20 g. paraffin oil at 270°, followed by heating 10 min. at 280°, gave 0.85 g. "linear" 2,8-dimethyl-4-hydroxy-6,7-benzoquinoline, yellow needles, m. 340° (decomposition) (after successive crystns. from C6H6, PhNO2, and EtOH), very soluble in 2 N NaOH, slightly soluble in hot 2 N HCl, showing marked

blue-green ultraviolet fluorescence in NaOH, blue in NaOH, and yellowish green in concentrated H2SO4. From 0.3 g. 2-C10H7NHNH2.HCl in 4 cc. MeOH with 0.2 cc. cyclohexanone, H. obtained a nearly quant. yield of 5,6-benzo-1,2,3,4-tetrahydrocarbazole (X), m. 137° (from MeOH); dark brown picrate, m. 192° (from C6H6). The formation of X is expedited by adding 2 N HCl to the original reaction mixture 1,2-MeC10H6NHAc, m. 193°, was hydrolyzed with HCl in alc. and 3.5 g. of the resulting salt in 25 cc. 7 N HCl was treated at 0° in 8 cc. H2O with 1.34 g. NaNO2, followed by treatment with urea and addition to 12 g. SnCl2 in 8 cc. HCl and 110 cc. H2O, giving a nearly quant. yield of 1-methyl-2-hydrazinonaphthalene-HCl (XI), leaflets (from HCl), m. 195° (decomposition), converted by AcONa into the free base, m. 110° (from MeOH), reducing Fehling solution XI with Me2CO gave 2,1-Me2C:NNHC10H6Me, leaflets, m. 99°. By heating 0.85 g. XI in 2 cc. AcOH with 1 cc. cyclohexanone and 20 mg. NiCl2 2 hrs. at 180°, and then 3 hrs. at 200°, a small amount of X was obtained, showing that ring closure had removed the 1-Me group. Careful warming of 135g. 3,6-(H2N)(O2N)C6H3Me with 125 g. arsenic acid, 270 g. glycerol, and 250 g. H2SO4 about 6 hrs. gave 108 g. of a difficultly separated mixture of 6-nitro-7-methylquinoline (XII) and its 5-Me isomer (XIII), from which 11.4 g. XIII, m. 165° (colorless HCl salt), was separated by successive crystns. from MeOH and Me2CO. Inasmuch as the components in the mother liquors from XIII could not be fractionally crystallized, the solution was evaporated,

treated with 350 cc. MeOH, and shaken 40 min. with 180 cc. hot 20% KOH in MeOH, followed by the addition of 700 cc. MeOH, yielding a highly insol. conversion product of XIII, the filtrate and washings from which gave 54 g. pure XII, colorless needles (from EtOH), m. 140°; colorless HCl salt. SnCl2 reduction of XIII yielded 6-amino-5-methylquinoline, coarse prisms, m. 163-4° (from C6H6) (yellow HCl salt; Ac derivative m. 168°), which when diazotized and poured into a Cu2O suspension in EtOH gave 5-methylquinoline, pale yellow oil (picrate m. 213-14°) (cf. Skraup and Brunner, Monatsh. 7, 141(1886)), 0.43 g. of which after treatment 10 hrs. with 0.65 g. CrO3 and 5 cc. 35% H2SO4 gave 5-carboxyquinoline, m. 330° (cf. Yakubovich, C.A.5,503). By a similar series of reactions XII gave the following: 6-amino-7-methylquinoline, plates, m. 139° (from C6H6); 7-methylquinoline (picrate, m. 235°, identical with that prepared from 3-MeC6H4NH2 by

the Skraup synthesis); 7-carboxyquinoline, m. 245°. XIII (1 g.) heated at the b.p. 3 min. with 12 cc. 10% KOH in MeOH gave 0.79 g. 1,2-bis(6-nitro-5-quinolyl)ethane, m. 300° (decomposition) (from AcOH), also formed when 2 N NaOH or alkaline arsenite solns. are used in place of KOH. The corresponding diamine, C20H18N4, formed greenish yellow needles (from C6H6) (properties not given). By analogous procedures H. obtained from 6-nitro-5,8-dimethylquinoline 1,2-bis(6-nitro-8-methyl-5-quinolyl)ethane, nearly colorless needles, m. 257° (from pyridine or AcOH), and from 5-nitro-8-methylquinoline 1,2-bis(5-nitro-8-quinolyl)ethane, needles, m. 221° (from C6H6 or AcOH), which on further treatment with alkali gave a deep violet color (cf. Trautmann, Ber. 23, 3673(1890)). 2-O2NC6H4Me in cooled absolute Et2O, treated with an equimol. amount of alc.-free EtOK in Et2O, the mixture let stand overnight, shaken with H2O, and the Et2O layer dried, filtered through Al2O3, and concentrated, gave 25-30% o,o'-dinitrobibenzyl, needles (from MeOH), m. 122°. Knuppel's reaction (cf. Ann. 310, 75(1900)), in which 6-nitroquinoline was heated with MeONa, gave 80% of a quinazone N-oxide (XIV), yellow needles, decomposing 330° (from AcOH) (red HCl salt (from H2O)), which when distilled with Fe powder gave the O-free quinazone, C18H10N4, pale yellow leaflets (from C6H6), m. 369°, sublimes undecompd. at 400°, gives a colorless HCl solution, and when heated with Zn dust, yields a bluish green semiquinone-like compound that may be reoxidized to the original quinazone by KMnO4. A reaction analogous to that giving XIV yielded from XII the 7,7'-di-Me derivative, yellow needles (from AcOH), m. 355° (decomposition), yielding, on reduction, the dimethylquinazone, C20H14N4, long, pale yellow needles, m. 380° (from xylene). Similarly 6-nitro-7,8-dimethylquinoline gave the corresponding tetra-Me derivative of XIV, yellowish green needles (from PhNO2), decomposing above 330° and forming, when distilled with Fe, the tetramethylquinazone, pale yellow needles, m. 354°.
6-Nitroquinoline (1 g.), 0.5 g. KCN, 15 cc. EtOH, 3 cc. H2O, and 0.5 g. KOH heated 4 hrs. gave 0.5 g. 5-cyano-6-ethoxyquinoline, needles, m. 130° (from MeOH), very resistant to HNO2, hot concentrated HCl, and cold H2SO4, whose colorless HCl and H2SO4 salts are difficultly soluble in H2O. By a similar reaction, using MeOH in place of EtOH, 5-cyano-6-methoxyquinoline, needles (from MeOH), m. 179°, was obtained. To a cooled mixture of 5 g. 6-nitroquinoline, 6 g. HONH2.HCl, and 90 cc. EtOH was added (in 1 portion) 30 cc. 20% KOH in MeOH. The exothermic reaction gave rise to 94% 5-amino-6-nitroquinoline (XV), yellow needles, m. 272° (yellow, difficultly soluble HCl salt), which with SnCl2 in HCl gave 5,6-diaminoquinoline chlorostannate; the latter, after detinning with H2S, yielded the HCl salt, pale yellow crystals, 0.1 g. of which when heated with 0.12 g. benzil in 5 cc. alc. and small amts. of AcONa gave the substituted quinoxaline, C23H15N3 (0.88 g.), plates from C6H6, m. 205°; the di-Ac derivative m. 252° with decomposition to form 5,6-(methylimidazolo)quinoline, m. 200° (hydrate, m. 70°).
The latter was more readily prepared by heating 0.5 g. XV in 5 cc. AcOH several hrs. with 2.1 g. SnCl2 in 4 cc. HCl, followed by detinning, evaporation, treatment with NH4OH, and extraction with Me2CO. Similarly, when XV was reduced in the presence of HCO2H (instead of AcOH), 5,6-imidazoloquinoline, m. 214° (from C6H6) (hydrate, m. 78°), was formed. By diazotization, the NH2 group in XV was replaced by iodine (using KI and Cu-bronze), yielding a resin which after trituration with HCl, extraction with NH4OHCHCl3, followed by washing with aqueous Na2SO4 and H2O, and passing the CHCl3 solution through Al2O3, gave red needles, which on repeated crystallization from MeOH and C6H6 yielded colorless 5-iodo-6-chloroquinoline, m. 136°. Deiodination with Cu-bronze in boiling PhNO2 gave 6,6'-dichloro-5,5'-biquinoline, colorless polyhedrons,

m. 205°. When, however, the iodine was removed by means of HI in AcOH, 5-iodo-6-chloroquinoline gave 6-chloroquinoline, m. 40-1°. Skraub's cyclization of 0.5 g. 5-nitro-6-aminoquinoline (Kaufmann and Zeller, C.A. 12, 1390), using arsenic acid gave 0.115 g. 4,7-phenanthroline, polyhedrons (from C6H6), m. 174° (showing only a faint ultraviolet fluorescence), also obtained (in 65% yield) by cyclization of 5-bromo-6-aminoquinoline. Evidently NO2 or Br in position 5 fails to block the formation of 4,7-phenanthroline. On the other hand, when 1 g. 6-acetamido-5-methylquinoline was heated gently 10-12 hrs. with 0.9 g. arsenic acid, 6 g. glycerol, 6 g. H2SO4, and 5 g. glacial AcOH, followed successively by treatment with H2O, extraction with NH4OH-CHCl3, extraction with 2 N HCl, reextn. with NH4OH-CHCl3, evaporation, treatment of the dry extract with 3 cc. pyridine and 0.2 g. 4-MeC6H4SO2Cl (to remove any unchanged starting product), and continued purification by extracting alternately with alkaline CHCl3 and HCl, filtering the CHCl3 solution through Al2O3, and finally subjecting the product to microdistn., using a water pump, H. obtained 3 fractions: (a) subliming 180°, (b) yellow oil, b. 200-20°, and (c) a red oil, b. 235°. Of these (b) gave 12 mg. linear 10-methyl-1,5-anthrazoline hydrate, C15H10N2.3H2O, felted needles, m. 62°, giving a yellow solution in acids and showing a brilliant bluish violet (ultraviolet) fluorescence. 8-Methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline (XVI), m. 225-6° (from EtOH), was prepared in 70% yield by heating 0.5 g. 6-hydrazino-8-methylquinoline (the synthesis of which is not given) with 3 cc. AcOH and 1.5 cc. cyclohexanone 6 hrs. and purifying the product by methods similar to those given above. XVI was also readily obtained in 75% yield by heating 0.33 g. of the substituted cyclohexanone hydrazone (XVII), m. 189°, at 200-240° with 15 mg. dry NiCl2, or (in only 34% yield) by heating this same hydrazone with 2 N H2SO4. The following steps also led to the formation of XVI: 4-nitro-2,5-xylidine → Skraup's synthesis 50% 6-nitro-5,8-dimethylquinoline, m. 118° (from alc.) → SnCl2 6-amino derivative, b12 194°, prisms, m. 175° → HCl salt, yellow → 7 N HCl+HNO2 diazo derivative → SnCl2 chlorostannate → H2S+HCl 85% 6-hydrazino-5,8-dimethylquinoline-HCl, yellow needles (free base (XVIII), m. 185°) → cyclohexanone 30% XVI. The ultraviolet absorption spectra of XVI prepared by the various methods were identical and showed a striking similarity to that of 7,8-dimethyl-10,11-tetramethylene-5,6(N)-pyrroquinoline. XVIII fails to undergo cyclization to XVI unless HCl is present. 6-Hydrazino-8-methylquinoline-HCl and MeCOEt in AcOH gave 40% 8,10,11-trimethyl-5,6(N)-pyrroquinoline, m. 188° (from EtOH), also formed in poor yield from the HCl salt of XVIII with concomitant removal of a Me group. Similarly, 0.5 g. 5-hydrazinoquinoline-HCl and cyclohexanone in AcOH gave 0.42 g. 10,11-tetramethylene-5(N),6-pyrroquinoline (XIX), m. 289° (from Me2CO). XIX was also isolated in 1-2% yield after extensive purification from 5-hydrazino-6-methylquinoline, m. 158° (pale yellow HCl salt).

SnCl2 reduction of 15 g. 6-nitro-2-hydroxylepidine gave 9.6 g. 2-hydroxy-4-methyl-6-aminoquinoline (XX), pale yellow, m. above 300°, cyclizing in the presence of arsenic acid, glycerol, and H2SO4-AcOH, followed by successive treatments with HCl and NH4OH, to form 2-hydroxy-4-methyl-4,7-phenanthroline (XXI), colorless prisms, the "angularity" of which was attested to by its very faint ultraviolet fluorescence, its ready solubility in aqueous NaOH and in boiling aqueous Na2CO3, and by the fact that its salts are colorless. 2,5-Xylidine, when heated at 160° with an equimol. amount of AcCH2CO2Et, gave the N-acetylacetyl derivative, m. 96° (from aqueous MeOH), which when heated 0.5 hr. on a steam bath with 6 parts concentrated H2SO4 gave (after pouring on ice) 90%

2-hydroxy-4,5,8-trimethylquinoline, m. 238° (from EtOH); 6-nitro derivative, pale yellow, m. 275° (from AcOH or EtOH); 6-amino derivative (XXII) (formed from the orange-red Sn double salt), pale yellow leaflets, m. 302° (from aqueous NH4OH or EtOH) (colorless HCl salt, difficultly soluble in H2O). The Skraup cyclization of XXII gave 2-hydroxy-4,9,10-trimethyl-1,5-anthrazoline (XXIII), pale yellow needles (from glacial AcOH or Ac2O), m. 290°, whose linear structure was indicated by the yellow color of its acid solns., its insoly. in alkali, and its strong blue ultraviolet fluorescence in MeOH. On diazotization, followed by SnCl2 reduction, XX gave 90% 2-hydroxy-4-methyl-6-hydrazinoquinoline, colorless needles from H2O, decomposing 240°, reducing Fehling solution in the cold, and forming a colorless HCl salt, which, when cyclized in the presence of MeCOEt and glacial AcOH, gave 90% 2-hydroxy-4,10,11-trimethyl-5,6(N)-pyrroquinoline, needles (from alc.), m. above 300° (decomposition); yellow HCl salt. When an analogous cyclization was carried out in the presence of cyclohexanone, 2-hydroxy-4-methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline, m. above 300°, was formed; golden yellow HCl salt. Diazotization of XXII, followed by reduction, gave the yellow chlorostannate of 2-hydroxy-4,5,8-trimethyl-6-hydrazinoquinoline, which in hot H2O, followed by filtration of the stannic acid, reacted with MeCOEt to form the corresponding substituted hydrazone, pale yellow needles, m. 112° (from a buffered AcONa solution), which failed to cyclize when treated with ZnCl2 at 200-60°, giving only 4,5,8-trimethylcarbostyril, m. 236°. Other attempts to cyclize the compound were equally unsuccessful. 2,3-Diphenyl-4,5-benzoindole, colorless prisms with blue-green iridescence, m. 166-7°, (3 g.) was formed from 1 g. 2-H2NC10H7, 0.5 g. C10H7NH2.HCl, and 2.2 g. benzoin at 140-65° (cf. Japp and Murray, J. Chemical Society 65, 889(1894)). 2,1-H2NC10H6Me subjected to a similar reaction gave 1-methyl-2-desylaminonaphthalene, 2,1-[PhC(OH):CPhNH]C10H6Me, pale yellow, m. 152-3° (from CHCl3-MeOH), which could not be cyclized by the use of ZnCl2, H2SO4, H3PO4, SnCl4, NiCl2, or SOCl2. The structure of this compound was shown by HClMeOH hydrolysis to benzoin and 2,1-H2NC10H6Me. The resonance energy of I was calculated from the total hydrogenation to decahydronaphthalene and also from its partial hydrogenation to tetrahydronaphthalene. The values obtained were, resp., 63.5 and 63.1 kcal./mol. and the approx. resonance energy per ring was 31.5 kcal. (cf. also Pauling, "Nature of the Chemical Bond," C.A. 33, 6700.4).

IT **86269-88-7**, 3H-Pyrrolo[3,2-f]quinolin-7-ol, 1,2,9-trimethyl- (preparation of)

RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)